Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 04:44 PM JST

PDB ID	:	5XXW
EMDB ID	:	EMD-6782
Title	:	GDP-microtubule complexed with KIF5C in ATP state
Authors	:	Morikawa, M.; Shigematsu, H.; Nitta, R.; Hirokawa, N.
Deposited on	:	2017-07-05
Resolution	:	6.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

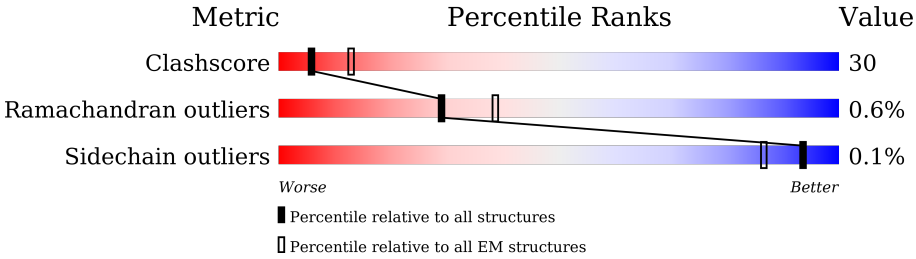
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	32% 71% 24% • •
1	C	438	32% 72% 23% • •
1	E	438	32% 73% 23% • •
1	G	438	36% 72% 23% • •
1	I	438	37% 71% 23% • •
1	K	438	36% 72% 23% • •
1	M	438	46% 75% 21% • •
1	O	438	46% 75% 21% • •

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Mol	Chain	Length	Quality of chain
1	Q	438	45% 75% 21%
2	B	426	28% 75% 21%
2	D	426	29% 77% 20%
2	F	426	29% 76% 21%
2	H	426	38% 79% 17%
2	J	426	38% 78% 18%
2	L	426	37% 79% 18%
2	N	426	32% 76% 20%
2	P	426	34% 74% 22%
2	R	426	33% 75% 21%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 60903 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3350	2121	570	638	21	0	0
1	C	428	3350	2121	570	638	21	0	0
1	E	428	3350	2121	570	638	21	0	0
1	G	428	3350	2121	570	638	21	0	0
1	I	428	3350	2121	570	638	21	0	0
1	K	428	3350	2121	570	638	21	0	0
1	M	428	3350	2121	570	638	21	0	0
1	O	428	3350	2121	570	638	21	0	0
1	Q	428	3350	2121	570	638	21	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3352	2105	575	647	25	0	0
2	D	426	3352	2105	575	647	25	0	0
2	F	426	3352	2105	575	647	25	0	0
2	H	426	3352	2105	575	647	25	0	0
2	J	426	3352	2105	575	647	25	0	0
2	L	426	3352	2105	575	647	25	0	0

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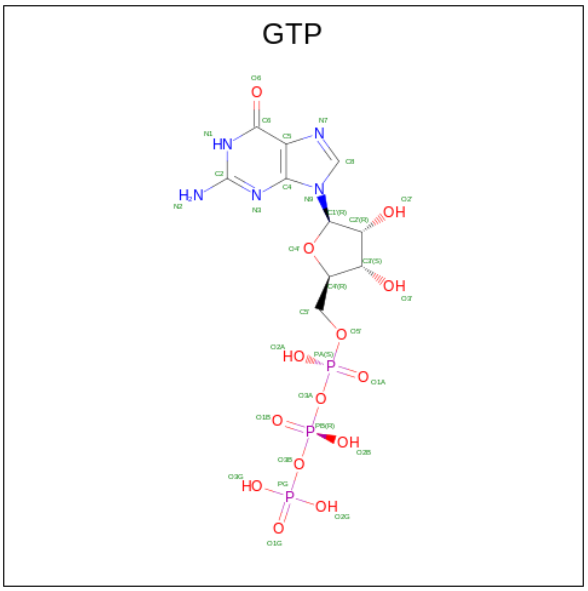
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	N	426	3352	2105	575	647	25	0	0
			Total	C	N	O	S		
2	P	426	3352	2105	575	647	25	0	0
			Total	C	N	O	S		
2	R	426	3352	2105	575	647	25	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	C	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	E	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	G	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	I	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	K	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	M	1	32	10	5	14	3	0
			Total	C	N	O	P	
3	O	1	32	10	5	14	3	0

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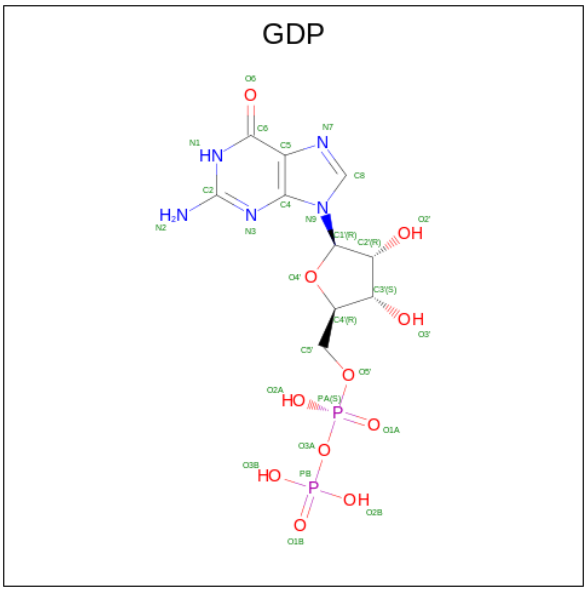
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	Q	1	32	10	5	14	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	C	1	1	1	0
4	E	1	1	1	0
4	G	1	1	1	0
4	I	1	1	1	0
4	K	1	1	1	0
4	M	1	1	1	0
4	O	1	1	1	0
4	Q	1	1	1	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	28	10	5	11	2	0
5	D	1	28	10	5	11	2	0
5	F	1	28	10	5	11	2	0
5	H	1	28	10	5	11	2	0
5	J	1	28	10	5	11	2	0
5	L	1	28	10	5	11	2	0
5	N	1	28	10	5	11	2	0
5	P	1	28	10	5	11	2	0
5	R	1	28	10	5	11	2	0

- Molecule 6 is water.

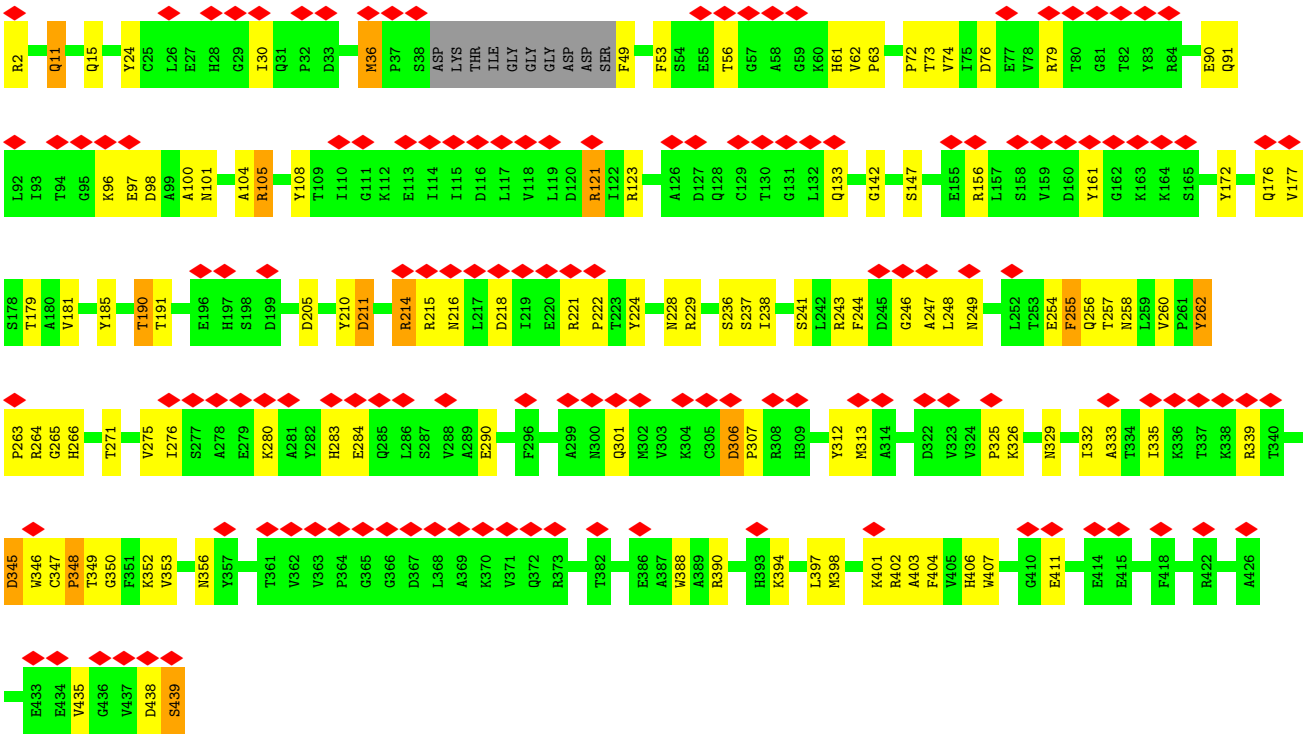
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	4	4	4	0
6	C	4	4	4	0
6	E	4	4	4	0
6	G	4	4	4	0
6	I	4	4	4	0
6	K	4	4	4	0
6	M	4	4	4	0
6	O	4	4	4	0
6	Q	4	4	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

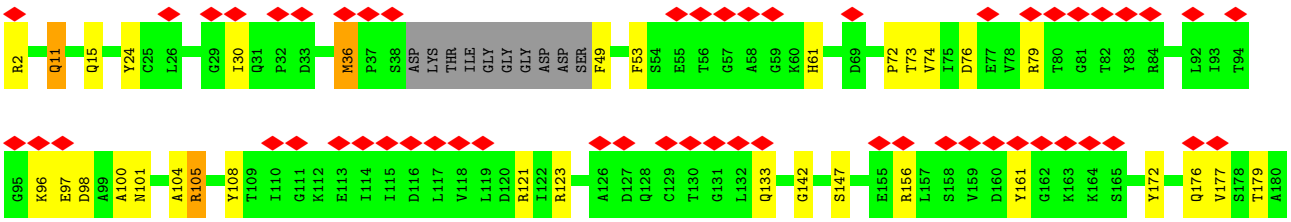
• Molecule 1: Tubulin alpha-1A chain

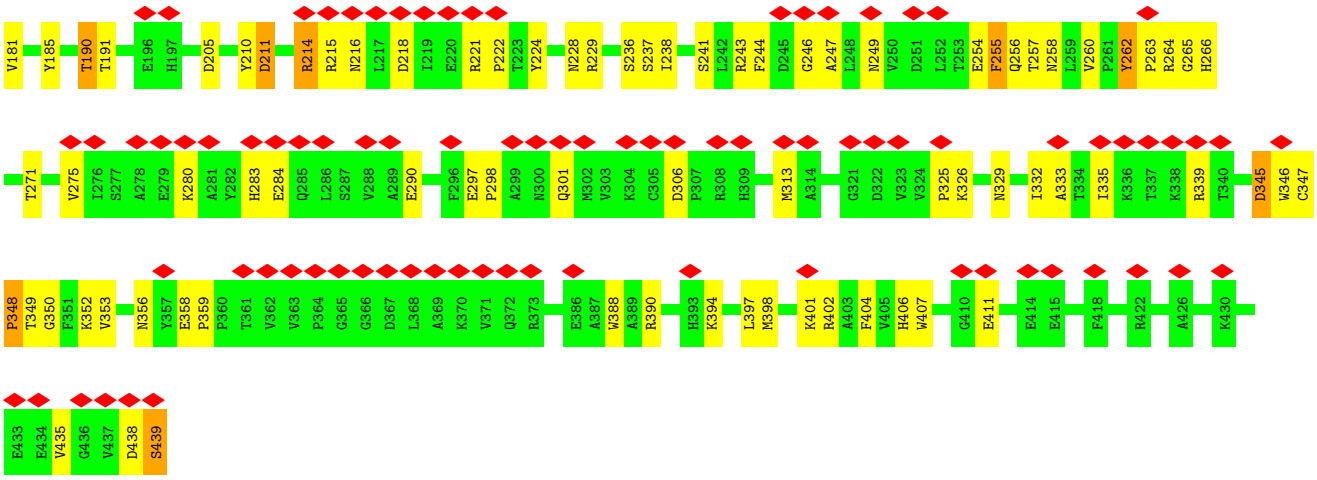
Chain A:



• Molecule 1: Tubulin alpha-1A chain

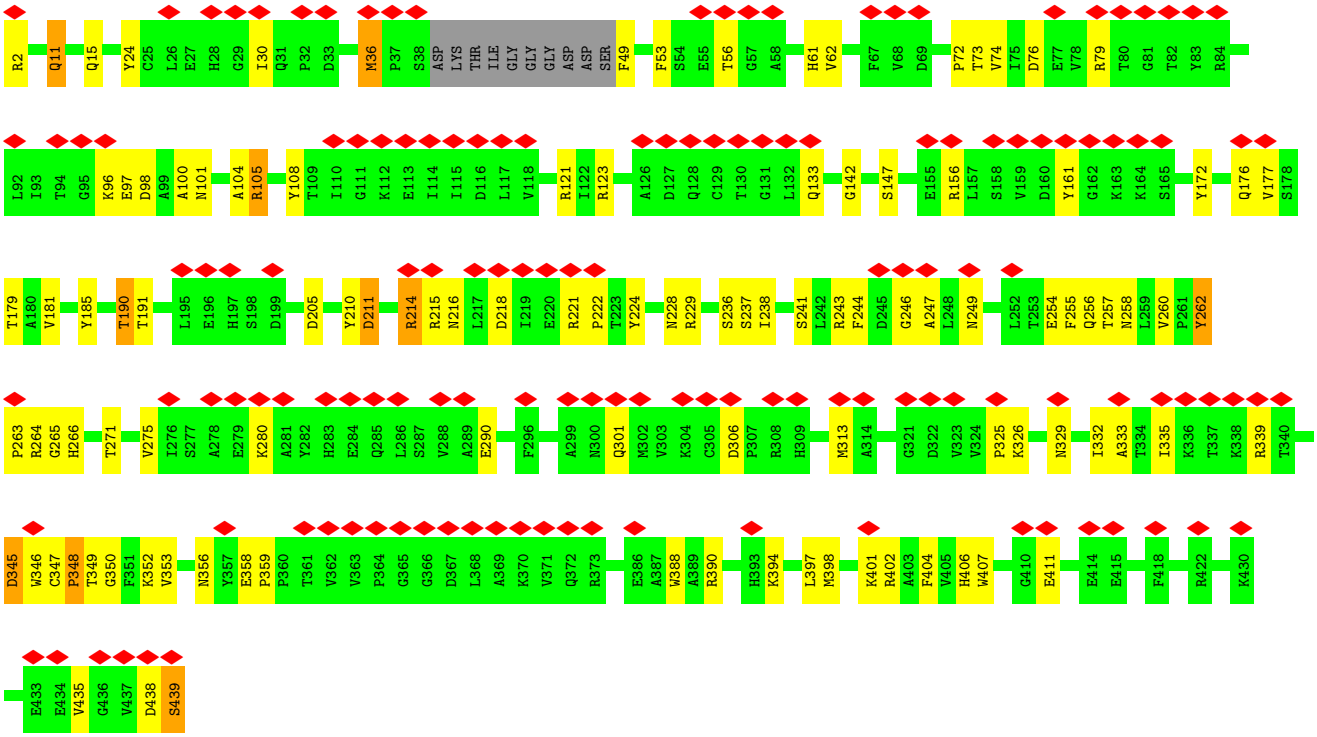
Chain C:





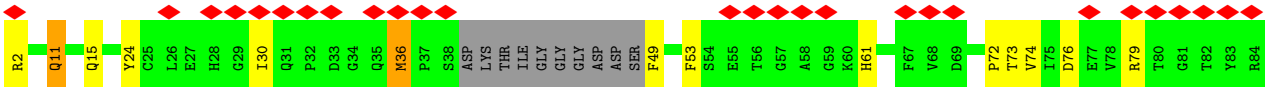
- Molecule 1: Tubulin alpha-1A chain

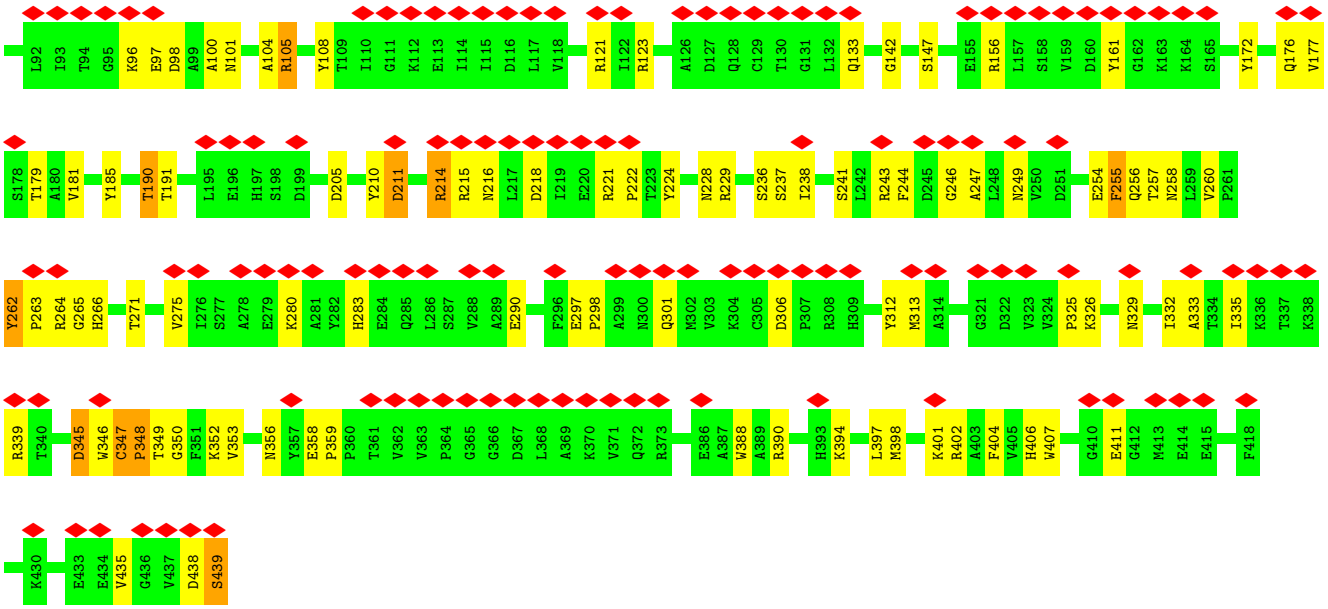
Chain E:



- Molecule 1: Tubulin alpha-1A chain

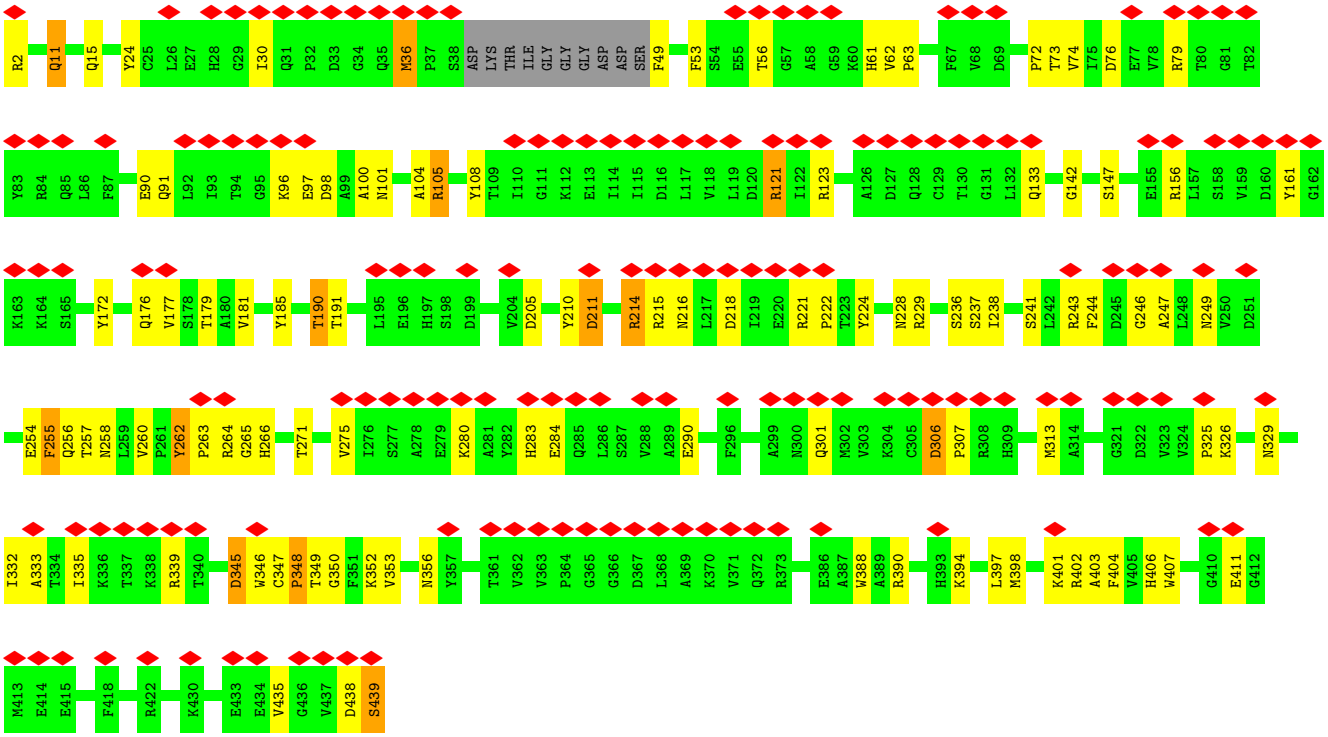
Chain G:





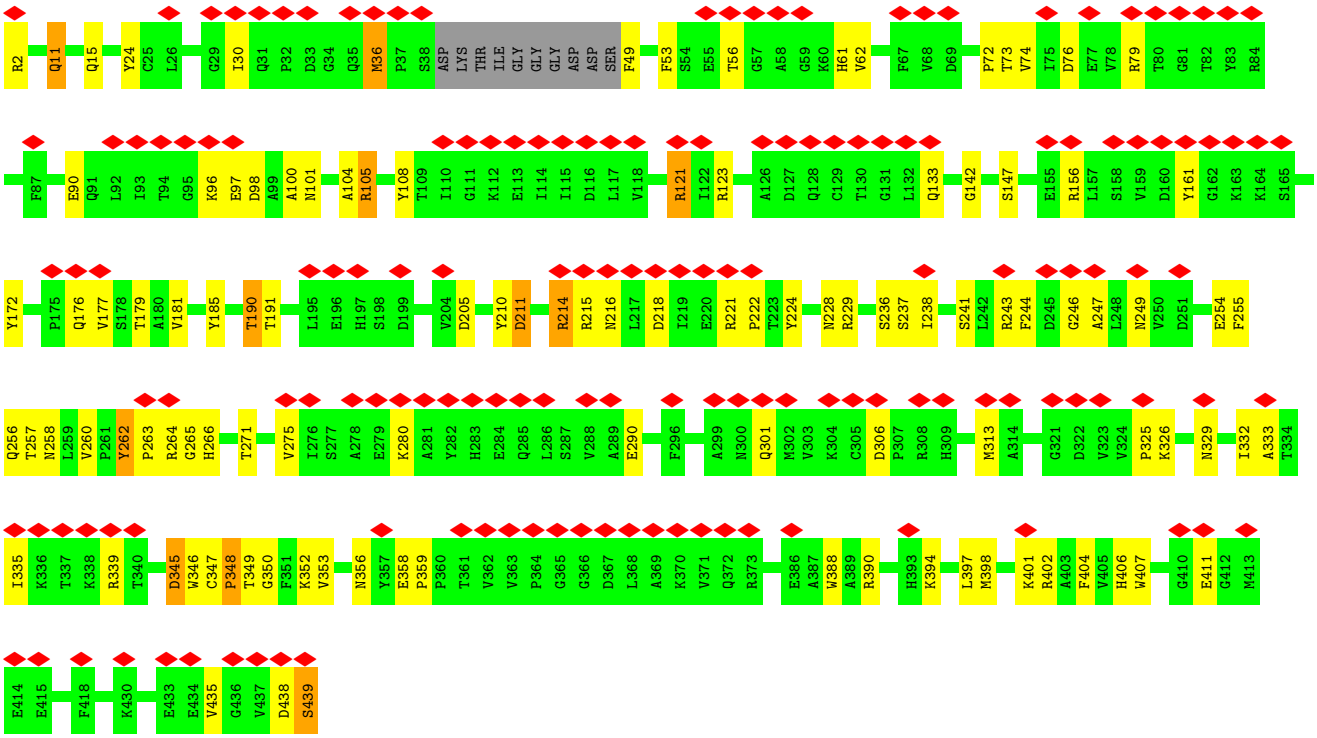
- Molecule 1: Tubulin alpha-1A chain

Chain I:



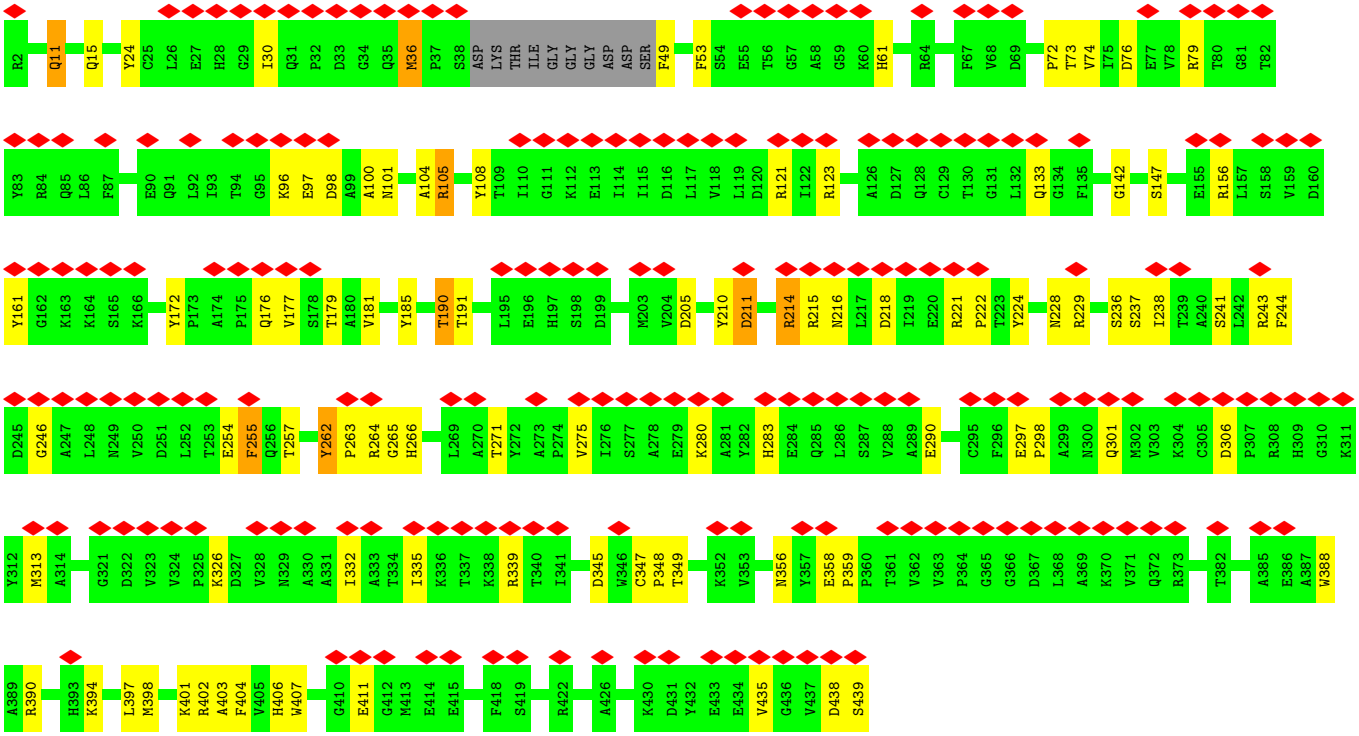
- Molecule 1: Tubulin alpha-1A chain

Chain K:



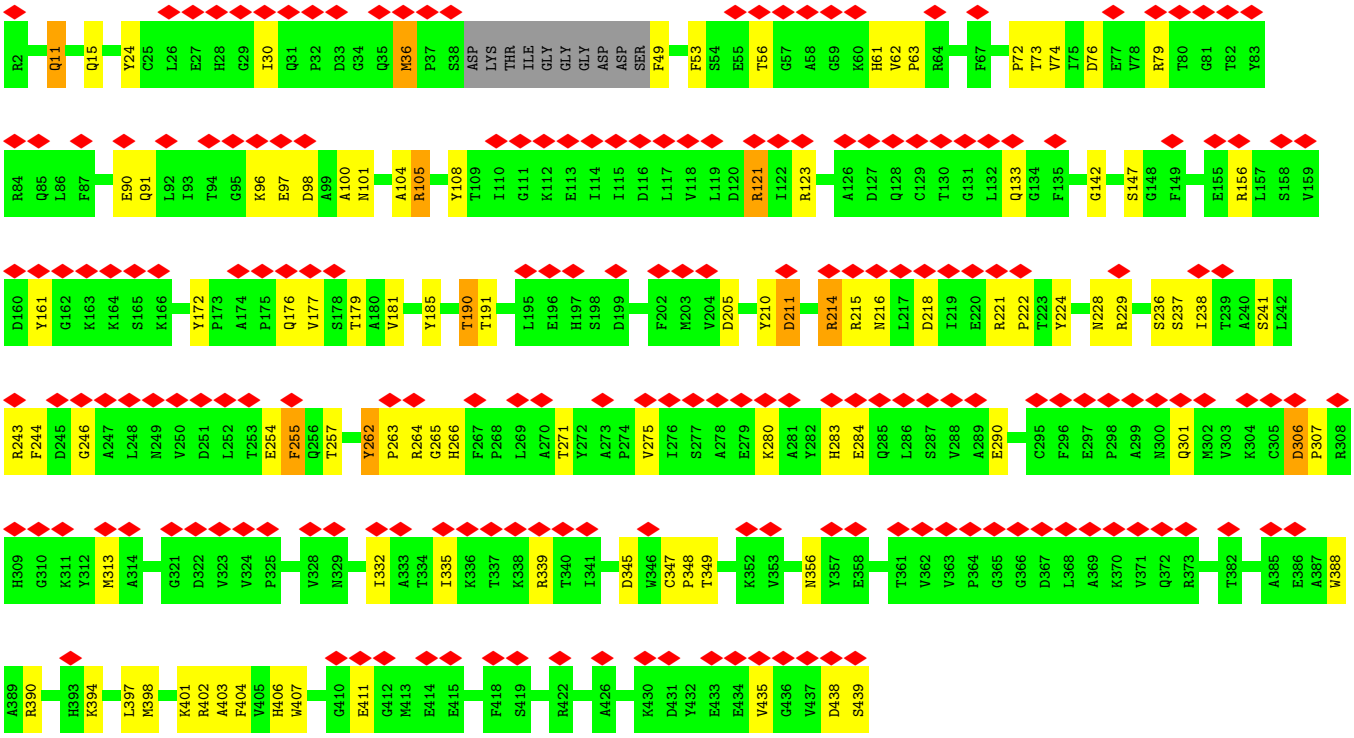
- Molecule 1: Tubulin alpha-1A chain

Chain M:



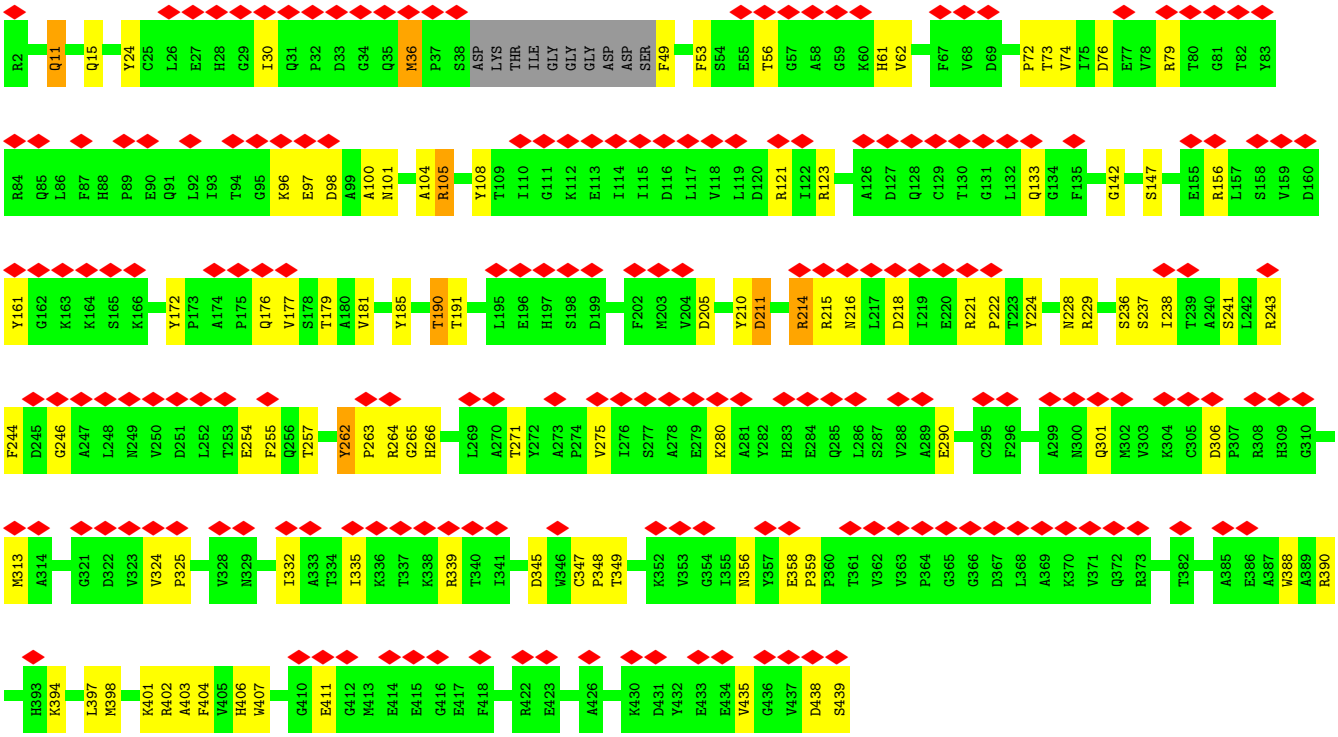
- Molecule 1: Tubulin alpha-1A chain

Chain O:



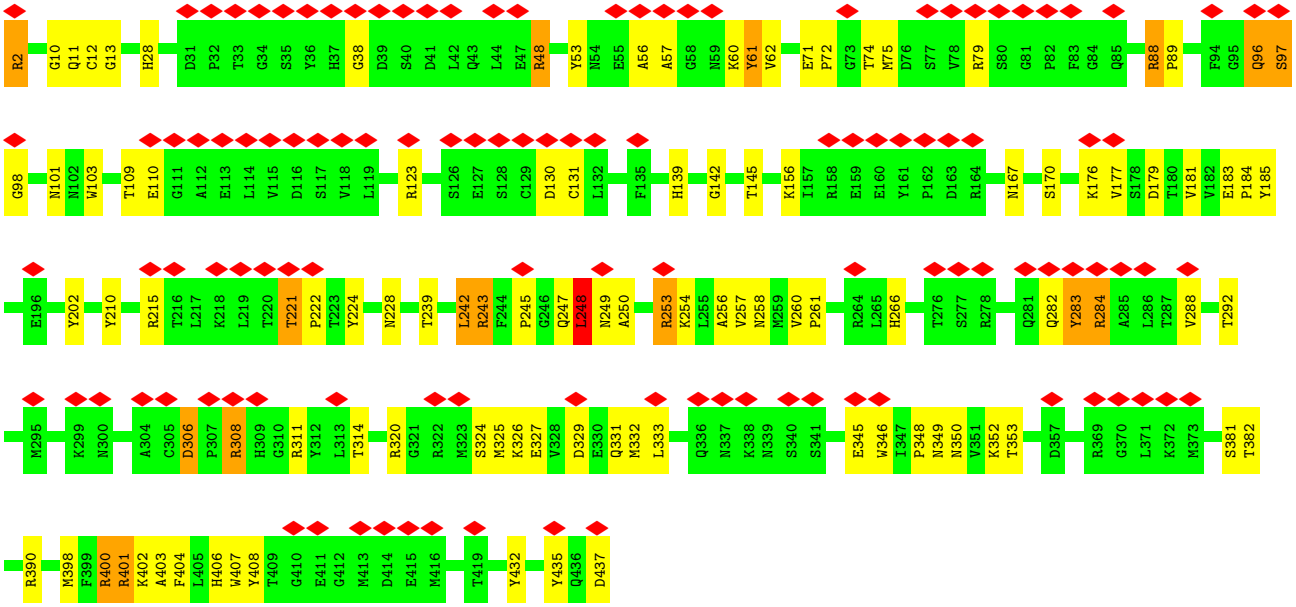
- Molecule 1: Tubulin alpha-1A chain

Chain Q:



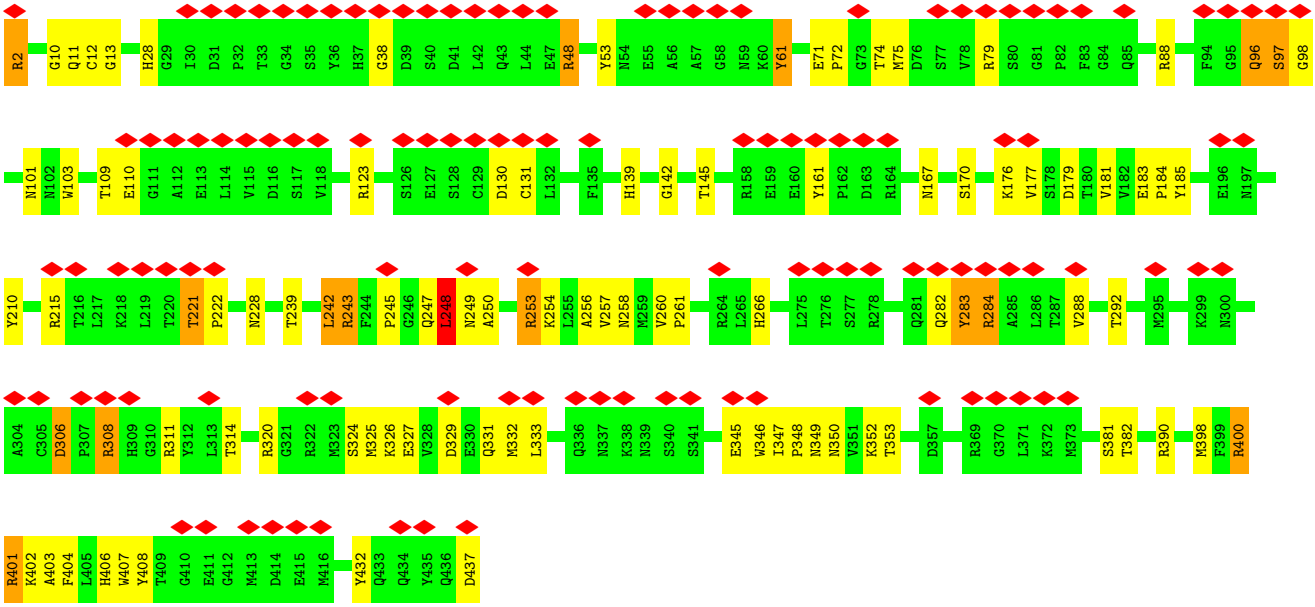
- Molecule 2: Tubulin beta chain

Chain B:



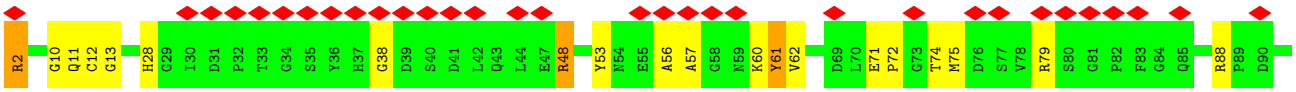
- Molecule 2: Tubulin beta chain

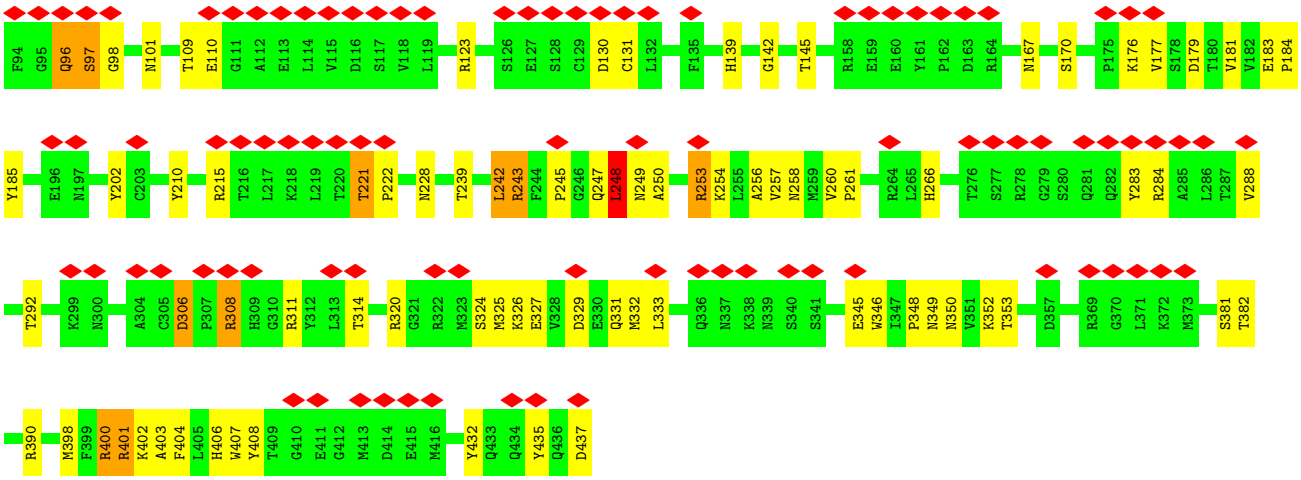
Chain D:



- Molecule 2: Tubulin beta chain

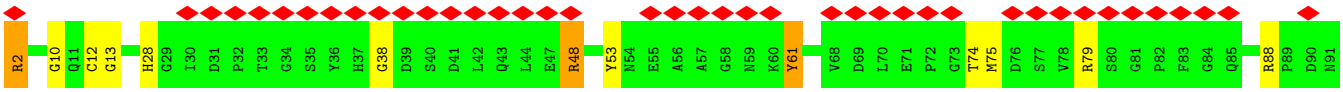
Chain F:

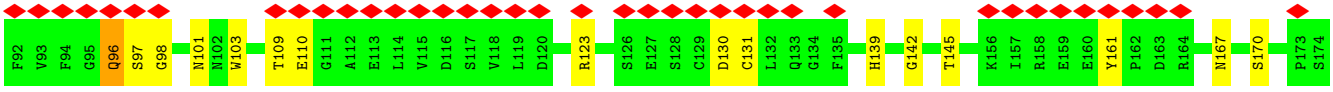


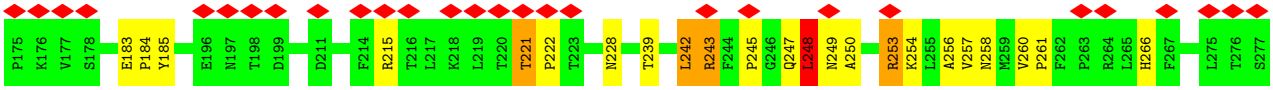


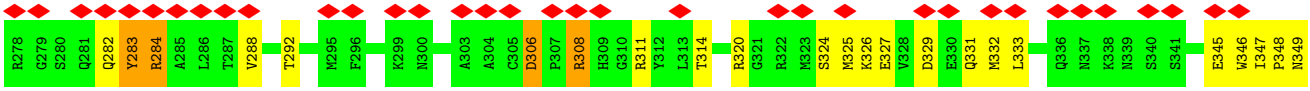
- Molecule 2: Tubulin beta chain

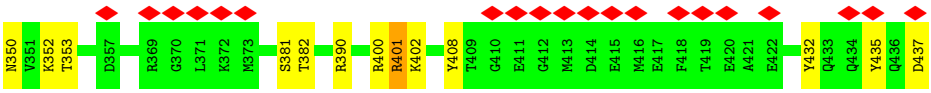
Chain H:





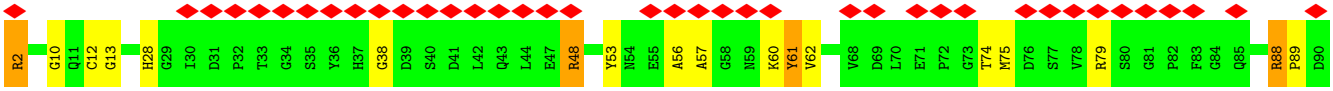


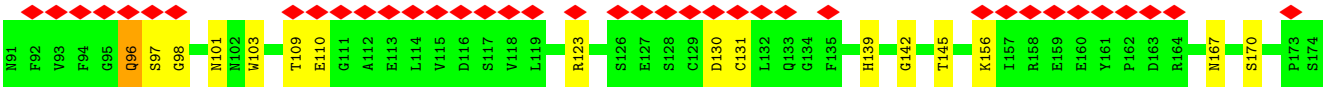


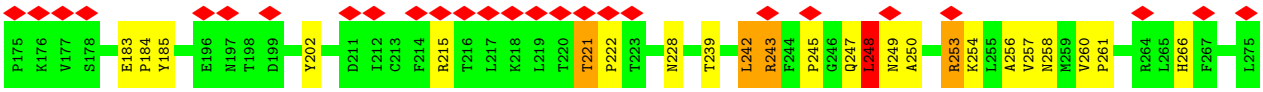


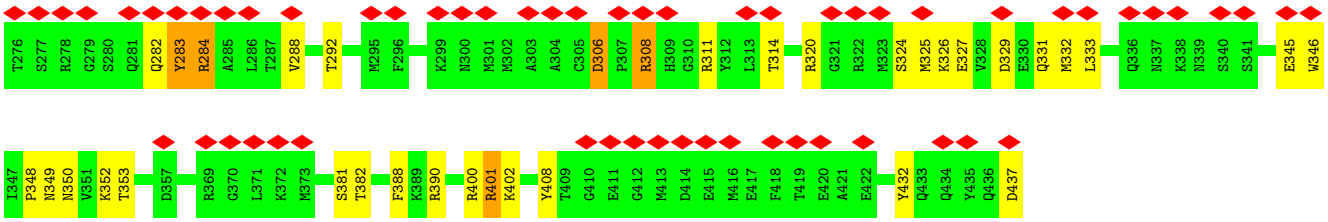
- Molecule 2: Tubulin beta chain

Chain J:



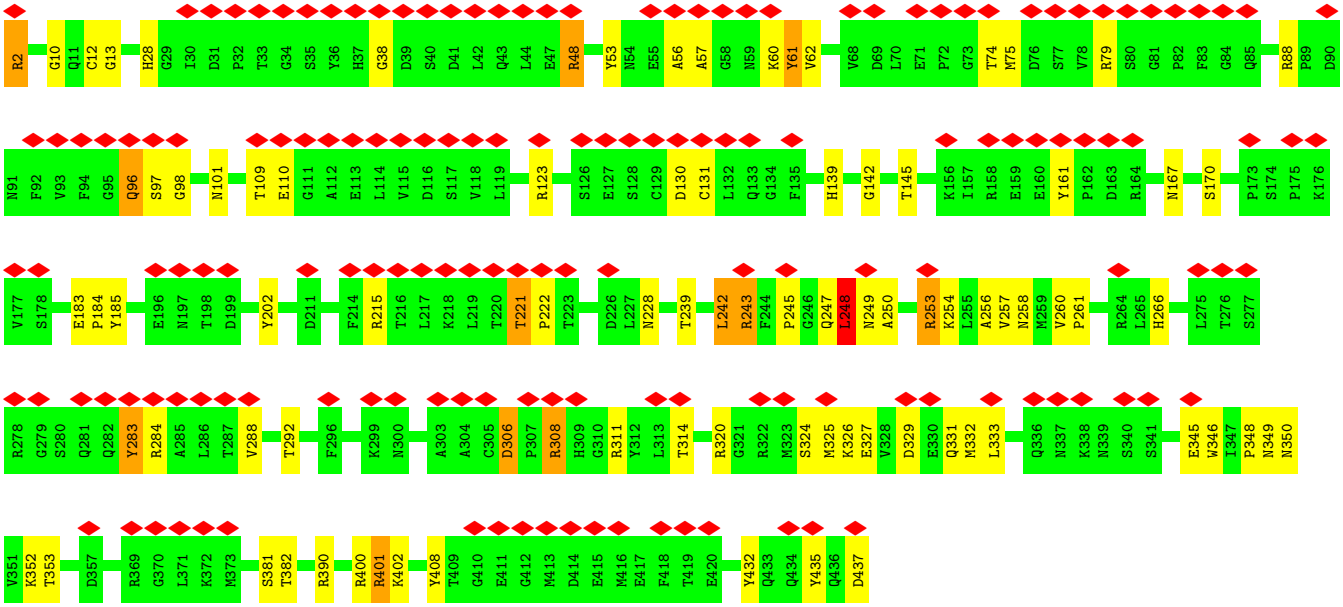






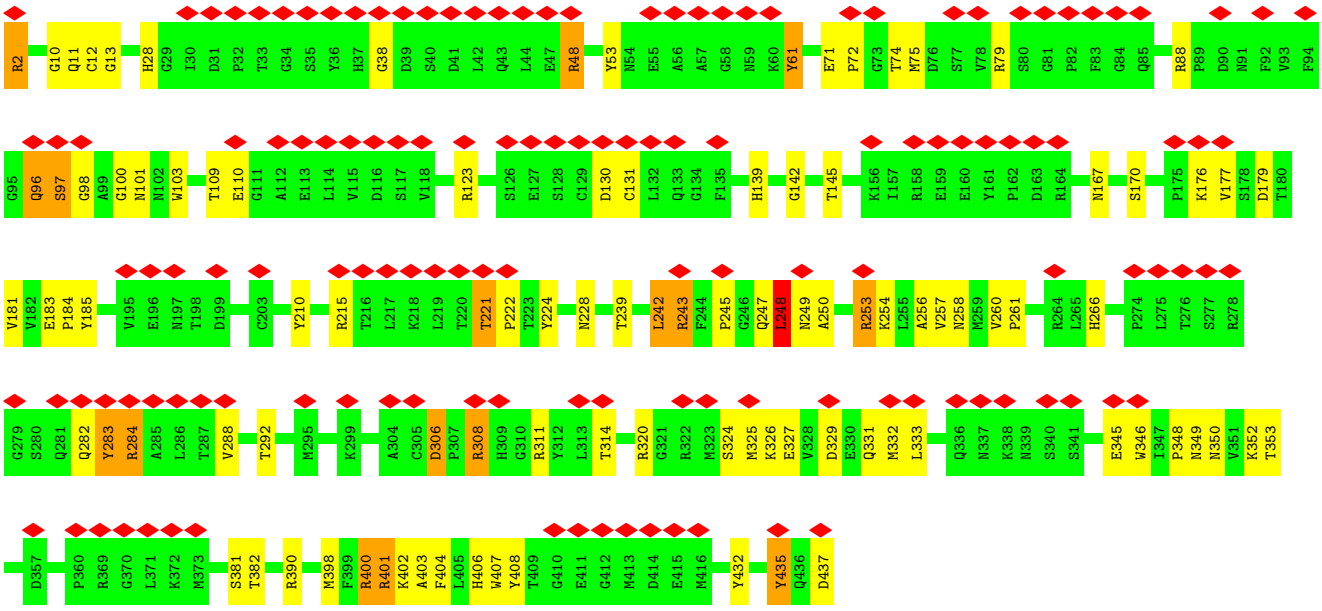
- Molecule 2: Tubulin beta chain

Chain L:



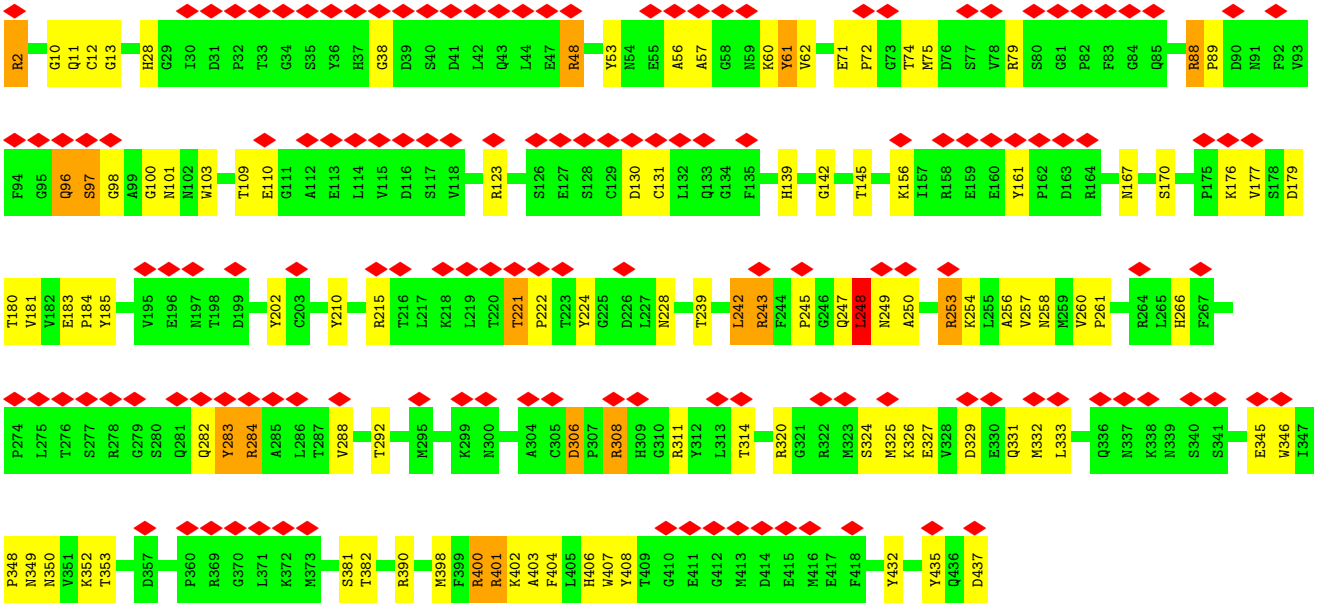
- Molecule 2: Tubulin beta chain

Chain N:



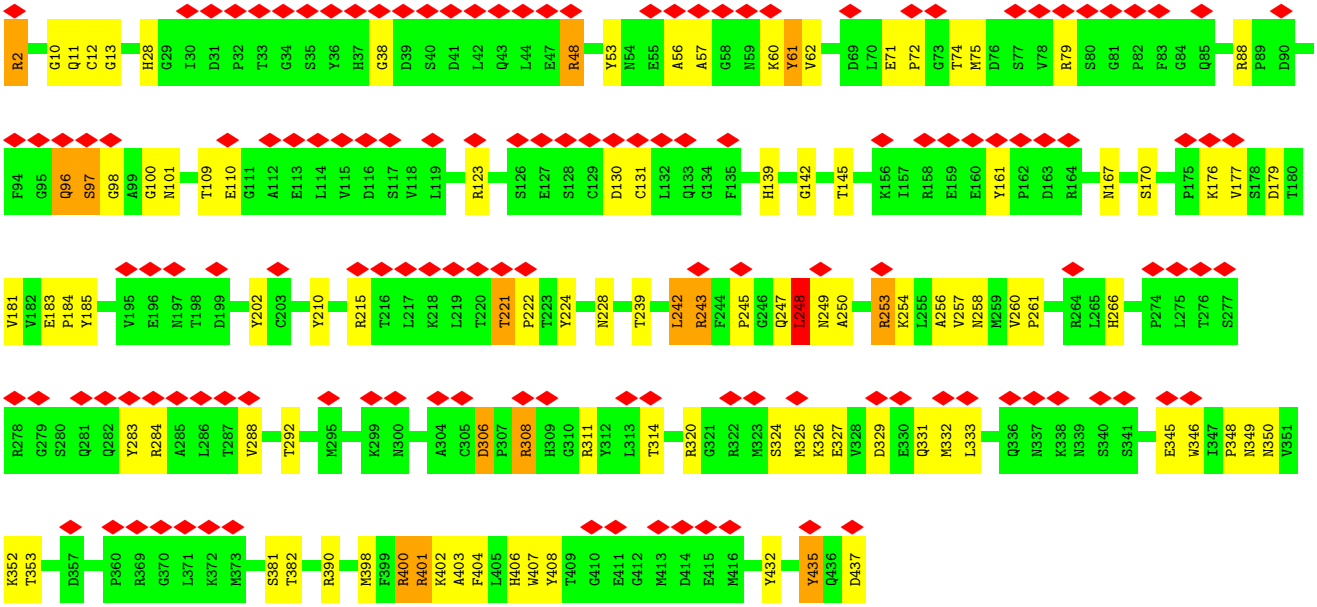
- Molecule 2: Tubulin beta chain

Chain P: 34% 74% 22% •



- Molecule 2: Tubulin beta chain

Chain R: 33% 75% 21% •



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7619°, rise=8.70662 Å, axial sym=C1	Depositor
Number of segments used	14302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	11.973	Depositor
Minimum map value	-2.929	Depositor
Average map value	0.777	Depositor
Map value standard deviation	2.451	Depositor
Recommended contour level	7.4	Depositor
Map size (Å)	246.52802, 246.52802, 282.48	wwPDB
Map dimensions	192, 192, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.14	10/3427 (0.3%)	1.44	45/4651 (1.0%)
1	C	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	E	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	G	1.14	10/3427 (0.3%)	1.44	45/4651 (1.0%)
1	I	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	K	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	M	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	O	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	Q	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
2	B	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	D	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	F	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	H	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	J	1.05	5/3427 (0.1%)	1.56	46/4642 (1.0%)
2	L	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	N	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	P	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	R	1.05	5/3427 (0.1%)	1.56	49/4642 (1.1%)
All	All	1.09	135/61686 (0.2%)	1.50	824/83637 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
All	All	0	9

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	265	GLY	CA-C	-15.06	1.27	1.51
1	Q	265	GLY	CA-C	-15.04	1.27	1.51
1	E	265	GLY	CA-C	-15.02	1.27	1.51
1	I	265	GLY	CA-C	-15.00	1.27	1.51
1	G	265	GLY	CA-C	-14.99	1.27	1.51
1	C	265	GLY	CA-C	-14.99	1.27	1.51
1	O	265	GLY	CA-C	-14.98	1.27	1.51
1	A	265	GLY	CA-C	-14.95	1.27	1.51
1	K	265	GLY	CA-C	-14.94	1.27	1.51
2	N	250	ALA	N-CA	-12.89	1.20	1.46
2	B	250	ALA	N-CA	-12.83	1.20	1.46
2	L	250	ALA	N-CA	-12.83	1.20	1.46
2	J	250	ALA	N-CA	-12.82	1.20	1.46
2	H	250	ALA	N-CA	-12.82	1.20	1.46
2	D	250	ALA	N-CA	-12.82	1.20	1.46
2	R	250	ALA	N-CA	-12.81	1.20	1.46
2	P	250	ALA	N-CA	-12.75	1.20	1.46
2	F	250	ALA	N-CA	-12.73	1.20	1.46
1	I	266	HIS	N-CA	-11.06	1.24	1.46
1	C	266	HIS	N-CA	-11.04	1.24	1.46
1	E	266	HIS	N-CA	-11.02	1.24	1.46
1	O	266	HIS	N-CA	-11.02	1.24	1.46
1	M	266	HIS	N-CA	-11.02	1.24	1.46
1	K	266	HIS	N-CA	-11.00	1.24	1.46
1	A	266	HIS	N-CA	-10.97	1.24	1.46
1	Q	266	HIS	N-CA	-10.97	1.24	1.46
1	G	266	HIS	N-CA	-10.96	1.24	1.46
1	K	265	GLY	N-CA	-8.71	1.32	1.46
1	C	265	GLY	N-CA	-8.69	1.33	1.46
1	I	265	GLY	N-CA	-8.69	1.33	1.46
1	G	265	GLY	N-CA	-8.68	1.33	1.46
1	M	265	GLY	N-CA	-8.67	1.33	1.46
1	A	265	GLY	N-CA	-8.61	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	265	GLY	N-CA	-8.61	1.33	1.46
1	Q	265	GLY	N-CA	-8.59	1.33	1.46
1	O	265	GLY	N-CA	-8.56	1.33	1.46
1	K	348	PRO	N-CA	-8.09	1.33	1.47
1	C	348	PRO	N-CA	-8.08	1.33	1.47
1	I	348	PRO	N-CA	-8.08	1.33	1.47
1	A	348	PRO	N-CA	-8.07	1.33	1.47
1	G	348	PRO	N-CA	-8.07	1.33	1.47
1	E	348	PRO	N-CA	-8.02	1.33	1.47
1	O	348	PRO	N-CA	-8.00	1.33	1.47
1	Q	348	PRO	N-CA	-7.99	1.33	1.47
1	M	348	PRO	N-CA	-7.98	1.33	1.47
1	E	264	ARG	CA-C	-7.66	1.33	1.52
1	K	264	ARG	CA-C	-7.62	1.33	1.52
1	G	264	ARG	CA-C	-7.61	1.33	1.52
1	Q	264	ARG	CA-C	-7.60	1.33	1.52
1	C	264	ARG	CA-C	-7.60	1.33	1.52
1	O	264	ARG	CA-C	-7.60	1.33	1.52
1	M	264	ARG	CA-C	-7.59	1.33	1.52
1	A	264	ARG	CA-C	-7.59	1.33	1.52
1	I	264	ARG	CA-C	-7.58	1.33	1.52
1	K	439	SER	N-CA	-7.37	1.31	1.46
1	M	439	SER	N-CA	-7.34	1.31	1.46
1	C	439	SER	N-CA	-7.34	1.31	1.46
1	I	439	SER	N-CA	-7.34	1.31	1.46
1	A	439	SER	N-CA	-7.32	1.31	1.46
1	G	439	SER	N-CA	-7.30	1.31	1.46
1	E	439	SER	N-CA	-7.29	1.31	1.46
1	Q	439	SER	N-CA	-7.28	1.31	1.46
1	O	439	SER	N-CA	-7.25	1.31	1.46
1	C	438	ASP	CA-C	-7.15	1.34	1.52
1	A	438	ASP	CA-C	-7.11	1.34	1.52
1	Q	348	PRO	CA-C	-7.11	1.38	1.52
1	G	438	ASP	CA-C	-7.10	1.34	1.52
1	M	438	ASP	CA-C	-7.10	1.34	1.52
1	K	438	ASP	CA-C	-7.09	1.34	1.52
1	O	438	ASP	CA-C	-7.08	1.34	1.52
1	E	438	ASP	CA-C	-7.08	1.34	1.52
1	Q	438	ASP	CA-C	-7.08	1.34	1.52
1	K	348	PRO	CA-C	-7.08	1.38	1.52
1	I	438	ASP	CA-C	-7.06	1.34	1.52
1	A	348	PRO	CA-C	-7.05	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	348	PRO	CA-C	-7.04	1.38	1.52
1	M	348	PRO	CA-C	-7.03	1.38	1.52
1	E	348	PRO	CA-C	-7.02	1.38	1.52
1	I	348	PRO	CA-C	-7.02	1.38	1.52
1	C	348	PRO	CA-C	-6.99	1.38	1.52
1	O	348	PRO	CA-C	-6.96	1.39	1.52
2	H	38	GLY	CA-C	-6.71	1.41	1.51
2	F	96	GLN	CA-C	-6.69	1.35	1.52
2	H	96	GLN	CA-C	-6.69	1.35	1.52
2	L	96	GLN	CA-C	-6.67	1.35	1.52
2	B	96	GLN	CA-C	-6.66	1.35	1.52
2	N	96	GLN	CA-C	-6.65	1.35	1.52
2	J	38	GLY	CA-C	-6.65	1.41	1.51
2	P	96	GLN	CA-C	-6.65	1.35	1.52
2	D	96	GLN	CA-C	-6.64	1.35	1.52
2	F	38	GLY	CA-C	-6.64	1.41	1.51
2	R	38	GLY	CA-C	-6.63	1.41	1.51
2	R	96	GLN	CA-C	-6.63	1.35	1.52
2	J	96	GLN	CA-C	-6.63	1.35	1.52
2	N	38	GLY	CA-C	-6.63	1.41	1.51
2	P	38	GLY	CA-C	-6.63	1.41	1.51
2	D	38	GLY	CA-C	-6.62	1.41	1.51
2	B	38	GLY	CA-C	-6.62	1.41	1.51
2	L	38	GLY	CA-C	-6.60	1.41	1.51
1	K	347	CYS	N-CA	-6.20	1.33	1.46
1	E	347	CYS	N-CA	-6.19	1.33	1.46
1	M	347	CYS	N-CA	-6.19	1.33	1.46
1	O	347	CYS	N-CA	-6.18	1.33	1.46
1	I	347	CYS	N-CA	-6.17	1.33	1.46
1	C	347	CYS	N-CA	-6.17	1.34	1.46
1	Q	347	CYS	N-CA	-6.16	1.34	1.46
1	A	347	CYS	N-CA	-6.11	1.34	1.46
1	G	347	CYS	N-CA	-6.11	1.34	1.46
2	D	97	SER	N-CA	-5.73	1.34	1.46
2	F	97	SER	N-CA	-5.70	1.34	1.46
2	B	242	LEU	N-CA	-5.69	1.34	1.46
2	B	97	SER	N-CA	-5.68	1.34	1.46
2	F	242	LEU	N-CA	-5.67	1.35	1.46
2	N	97	SER	N-CA	-5.67	1.35	1.46
2	H	97	SER	N-CA	-5.67	1.35	1.46
2	N	242	LEU	N-CA	-5.67	1.35	1.46
2	P	97	SER	N-CA	-5.66	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	242	LEU	N-CA	-5.66	1.35	1.46
2	H	242	LEU	N-CA	-5.65	1.35	1.46
2	R	97	SER	N-CA	-5.65	1.35	1.46
2	J	97	SER	N-CA	-5.65	1.35	1.46
2	D	242	LEU	N-CA	-5.64	1.35	1.46
2	R	242	LEU	N-CA	-5.64	1.35	1.46
2	L	97	SER	N-CA	-5.64	1.35	1.46
2	L	242	LEU	N-CA	-5.64	1.35	1.46
2	J	242	LEU	N-CA	-5.62	1.35	1.46
1	Q	49	PHE	N-CA	-5.16	1.36	1.46
1	E	49	PHE	N-CA	-5.16	1.36	1.46
1	K	49	PHE	N-CA	-5.13	1.36	1.46
1	I	49	PHE	N-CA	-5.12	1.36	1.46
1	M	49	PHE	N-CA	-5.09	1.36	1.46
1	O	49	PHE	N-CA	-5.09	1.36	1.46
1	G	49	PHE	N-CA	-5.08	1.36	1.46
1	A	49	PHE	N-CA	-5.06	1.36	1.46
1	C	49	PHE	N-CA	-5.01	1.36	1.46

All (824) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	48	ARG	NE-CZ-NH1	20.40	130.50	120.30
2	R	48	ARG	NE-CZ-NH1	20.36	130.48	120.30
2	P	48	ARG	NE-CZ-NH1	20.32	130.46	120.30
2	B	48	ARG	NE-CZ-NH1	20.28	130.44	120.30
2	D	48	ARG	NE-CZ-NH1	20.18	130.39	120.30
2	N	48	ARG	NE-CZ-NH1	20.18	130.39	120.30
2	F	48	ARG	NE-CZ-NH1	20.17	130.39	120.30
2	J	48	ARG	NE-CZ-NH1	20.17	130.38	120.30
2	L	48	ARG	NE-CZ-NH1	20.14	130.37	120.30
2	R	2	ARG	NE-CZ-NH1	17.74	129.17	120.30
2	N	2	ARG	NE-CZ-NH1	17.72	129.16	120.30
2	H	2	ARG	NE-CZ-NH1	17.72	129.16	120.30
2	F	2	ARG	NE-CZ-NH1	17.66	129.13	120.30
2	P	2	ARG	NE-CZ-NH1	17.65	129.12	120.30
2	J	2	ARG	NE-CZ-NH1	17.63	129.11	120.30
2	D	2	ARG	NE-CZ-NH1	17.61	129.11	120.30
2	L	2	ARG	NE-CZ-NH1	17.59	129.10	120.30
2	B	2	ARG	NE-CZ-NH1	17.57	129.09	120.30
2	F	308	ARG	NE-CZ-NH2	-17.28	111.66	120.30
2	L	308	ARG	NE-CZ-NH2	-17.26	111.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	88	ARG	NE-CZ-NH1	17.21	128.91	120.30
2	J	308	ARG	NE-CZ-NH2	-17.19	111.70	120.30
2	L	88	ARG	NE-CZ-NH1	17.18	128.89	120.30
2	P	308	ARG	NE-CZ-NH2	-17.15	111.73	120.30
2	B	308	ARG	NE-CZ-NH2	-17.12	111.74	120.30
2	R	308	ARG	NE-CZ-NH2	-17.11	111.75	120.30
2	N	88	ARG	NE-CZ-NH1	17.10	128.85	120.30
2	D	308	ARG	NE-CZ-NH2	-17.10	111.75	120.30
2	B	88	ARG	NE-CZ-NH1	17.08	128.84	120.30
2	H	308	ARG	NE-CZ-NH2	-17.02	111.79	120.30
2	P	88	ARG	NE-CZ-NH1	17.02	128.81	120.30
2	N	308	ARG	NE-CZ-NH2	-17.02	111.79	120.30
2	H	88	ARG	NE-CZ-NH1	16.98	128.79	120.30
2	R	88	ARG	NE-CZ-NH1	16.96	128.78	120.30
2	F	88	ARG	NE-CZ-NH1	16.94	128.77	120.30
2	J	88	ARG	NE-CZ-NH1	16.88	128.74	120.30
2	R	48	ARG	NE-CZ-NH2	-14.44	113.08	120.30
2	B	48	ARG	NE-CZ-NH2	-14.37	113.12	120.30
2	D	48	ARG	NE-CZ-NH2	-14.30	113.15	120.30
2	F	48	ARG	NE-CZ-NH2	-14.29	113.15	120.30
2	H	48	ARG	NE-CZ-NH2	-14.27	113.17	120.30
2	P	48	ARG	NE-CZ-NH2	-14.25	113.18	120.30
2	J	48	ARG	NE-CZ-NH2	-14.24	113.18	120.30
2	L	48	ARG	NE-CZ-NH2	-14.24	113.18	120.30
2	N	48	ARG	NE-CZ-NH2	-14.20	113.20	120.30
2	H	88	ARG	NE-CZ-NH2	-13.75	113.43	120.30
2	L	88	ARG	NE-CZ-NH2	-13.73	113.43	120.30
2	B	88	ARG	NE-CZ-NH2	-13.73	113.44	120.30
2	N	88	ARG	NE-CZ-NH2	-13.65	113.48	120.30
2	F	88	ARG	NE-CZ-NH2	-13.64	113.48	120.30
2	R	88	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	M	105	ARG	NE-CZ-NH2	-13.57	113.52	120.30
2	D	88	ARG	NE-CZ-NH2	-13.53	113.54	120.30
1	K	105	ARG	NE-CZ-NH2	-13.50	113.55	120.30
2	P	88	ARG	NE-CZ-NH2	-13.48	113.56	120.30
1	I	105	ARG	NE-CZ-NH2	-13.44	113.58	120.30
2	J	88	ARG	NE-CZ-NH2	-13.43	113.59	120.30
1	E	105	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	A	105	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	O	105	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	C	105	ARG	NE-CZ-NH2	-13.33	113.64	120.30
2	H	400	ARG	NE-CZ-NH2	13.28	126.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	105	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	Q	105	ARG	NE-CZ-NH2	-13.26	113.67	120.30
2	L	400	ARG	NE-CZ-NH2	13.20	126.90	120.30
2	B	400	ARG	NE-CZ-NH2	13.17	126.88	120.30
2	R	400	ARG	NE-CZ-NH2	13.12	126.86	120.30
2	P	400	ARG	NE-CZ-NH2	13.08	126.84	120.30
2	F	400	ARG	NE-CZ-NH2	13.07	126.84	120.30
2	J	400	ARG	NE-CZ-NH2	13.06	126.83	120.30
2	N	400	ARG	NE-CZ-NH2	13.03	126.82	120.30
2	D	400	ARG	NE-CZ-NH2	12.94	126.77	120.30
2	H	283	TYR	CB-CG-CD1	-12.64	113.42	121.00
2	B	283	TYR	CB-CG-CD1	-12.62	113.43	121.00
2	L	283	TYR	CB-CG-CD1	-12.56	113.47	121.00
2	R	283	TYR	CB-CG-CD1	-12.51	113.50	121.00
2	J	215	ARG	NE-CZ-NH2	-12.51	114.05	120.30
2	D	283	TYR	CB-CG-CD1	-12.50	113.50	121.00
2	F	215	ARG	NE-CZ-NH2	-12.49	114.06	120.30
2	L	215	ARG	NE-CZ-NH2	-12.48	114.06	120.30
2	P	283	TYR	CB-CG-CD1	-12.48	113.51	121.00
2	B	215	ARG	NE-CZ-NH2	-12.46	114.07	120.30
2	F	283	TYR	CB-CG-CD1	-12.44	113.54	121.00
2	R	215	ARG	NE-CZ-NH2	-12.43	114.09	120.30
2	N	283	TYR	CB-CG-CD1	-12.42	113.55	121.00
2	J	283	TYR	CB-CG-CD1	-12.39	113.57	121.00
2	D	215	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	N	215	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	P	215	ARG	NE-CZ-NH2	-12.35	114.12	120.30
2	H	215	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	E	123	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	M	123	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	O	123	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	Q	123	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	K	123	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	C	123	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	A	123	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	I	123	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	G	123	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	O	215	ARG	NE-CZ-NH1	11.33	125.97	120.30
1	C	215	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	Q	215	ARG	NE-CZ-NH1	11.25	125.93	120.30
1	I	214	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	E	214	ARG	NE-CZ-NH2	-11.23	114.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	215	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	I	215	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	G	215	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	215	ARG	NE-CZ-NH1	11.19	125.90	120.30
1	A	214	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	Q	214	ARG	NE-CZ-NH2	-11.15	114.73	120.30
1	G	214	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	M	215	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	K	214	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	M	214	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	O	214	ARG	NE-CZ-NH2	-11.10	114.75	120.30
2	D	284	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	E	215	ARG	NE-CZ-NH1	11.08	125.84	120.30
2	L	284	ARG	NE-CZ-NH1	11.08	125.84	120.30
2	H	284	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	B	284	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	C	214	ARG	NE-CZ-NH2	-11.01	114.80	120.30
2	P	284	ARG	NE-CZ-NH1	11.00	125.80	120.30
2	J	284	ARG	NE-CZ-NH1	10.96	125.78	120.30
2	F	284	ARG	NE-CZ-NH1	10.96	125.78	120.30
2	N	284	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	I	390	ARG	NE-CZ-NH1	10.93	125.77	120.30
2	R	284	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	Q	390	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	E	390	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	265	GLY	CA-C-N	-10.84	93.35	117.20
1	O	390	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	Q	265	GLY	CA-C-N	-10.82	93.40	117.20
1	K	265	GLY	CA-C-N	-10.80	93.45	117.20
1	C	390	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	G	265	GLY	CA-C-N	-10.78	93.49	117.20
1	E	265	GLY	CA-C-N	-10.78	93.50	117.20
1	M	265	GLY	CA-C-N	-10.78	93.49	117.20
1	C	265	GLY	CA-C-N	-10.76	93.52	117.20
1	O	265	GLY	CA-C-N	-10.76	93.53	117.20
1	I	265	GLY	CA-C-N	-10.76	93.54	117.20
1	A	390	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	K	390	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	G	390	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	M	390	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	Q	36	MET	CG-SD-CE	10.03	116.25	100.20
1	A	36	MET	CG-SD-CE	10.00	116.20	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	36	MET	CG-SD-CE	9.99	116.19	100.20
1	C	36	MET	CG-SD-CE	9.99	116.18	100.20
1	E	36	MET	CG-SD-CE	9.98	116.17	100.20
1	I	36	MET	CG-SD-CE	9.98	116.17	100.20
1	G	36	MET	CG-SD-CE	9.97	116.15	100.20
1	K	36	MET	CG-SD-CE	9.97	116.15	100.20
1	O	36	MET	CG-SD-CE	9.95	116.12	100.20
1	G	264	ARG	C-N-CA	-9.93	101.46	122.30
1	E	264	ARG	C-N-CA	-9.92	101.48	122.30
1	O	264	ARG	C-N-CA	-9.90	101.51	122.30
1	K	264	ARG	C-N-CA	-9.89	101.52	122.30
1	C	264	ARG	C-N-CA	-9.89	101.53	122.30
1	M	264	ARG	C-N-CA	-9.89	101.53	122.30
1	Q	264	ARG	C-N-CA	-9.88	101.54	122.30
1	A	264	ARG	C-N-CA	-9.88	101.55	122.30
1	I	264	ARG	C-N-CA	-9.87	101.58	122.30
2	H	243	ARG	NE-CZ-NH1	9.58	125.09	120.30
2	L	401	ARG	NE-CZ-NH2	9.54	125.07	120.30
2	H	401	ARG	NE-CZ-NH2	9.52	125.06	120.30
2	F	401	ARG	NE-CZ-NH2	9.51	125.05	120.30
2	R	243	ARG	NE-CZ-NH1	9.49	125.05	120.30
2	R	401	ARG	NE-CZ-NH2	9.49	125.04	120.30
2	N	401	ARG	NE-CZ-NH2	9.45	125.03	120.30
2	B	243	ARG	NE-CZ-NH1	9.43	125.01	120.30
2	P	401	ARG	NE-CZ-NH2	9.42	125.01	120.30
2	J	401	ARG	NE-CZ-NH2	9.41	125.00	120.30
2	D	401	ARG	NE-CZ-NH2	9.41	125.00	120.30
2	H	283	TYR	CB-CG-CD2	9.39	126.63	121.00
2	P	243	ARG	NE-CZ-NH1	9.39	125.00	120.30
2	D	243	ARG	NE-CZ-NH1	9.39	124.99	120.30
2	F	243	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	B	283	TYR	CB-CG-CD2	9.33	126.60	121.00
2	L	243	ARG	NE-CZ-NH1	9.32	124.96	120.30
2	N	243	ARG	NE-CZ-NH1	9.31	124.96	120.30
2	B	401	ARG	NE-CZ-NH2	9.28	124.94	120.30
2	N	283	TYR	CB-CG-CD2	9.27	126.56	121.00
2	P	283	TYR	CB-CG-CD2	9.27	126.56	121.00
2	J	243	ARG	NE-CZ-NH1	9.26	124.93	120.30
2	L	283	TYR	CB-CG-CD2	9.26	126.56	121.00
2	J	283	TYR	CB-CG-CD2	9.24	126.55	121.00
2	F	283	TYR	CB-CG-CD2	9.21	126.52	121.00
2	D	283	TYR	CB-CG-CD2	9.19	126.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	283	TYR	CB-CG-CD2	9.17	126.50	121.00
1	A	265	GLY	O-C-N	9.06	137.19	122.70
1	G	265	GLY	O-C-N	9.05	137.19	122.70
1	K	265	GLY	O-C-N	9.04	137.17	122.70
1	I	265	GLY	O-C-N	9.04	137.16	122.70
1	M	265	GLY	O-C-N	9.03	137.15	122.70
1	Q	265	GLY	O-C-N	9.04	137.16	122.70
2	H	185	TYR	CB-CG-CD2	-9.02	115.59	121.00
1	C	265	GLY	O-C-N	9.01	137.11	122.70
1	E	265	GLY	O-C-N	9.00	137.09	122.70
1	O	265	GLY	O-C-N	8.99	137.09	122.70
2	L	185	TYR	CB-CG-CD2	-8.99	115.61	121.00
2	R	185	TYR	CB-CG-CD2	-8.98	115.61	121.00
2	N	185	TYR	CB-CG-CD2	-8.96	115.62	121.00
2	D	185	TYR	CB-CG-CD2	-8.96	115.62	121.00
2	F	185	TYR	CB-CG-CD2	-8.94	115.64	121.00
2	P	185	TYR	CB-CG-CD2	-8.84	115.69	121.00
2	J	185	TYR	CB-CG-CD2	-8.83	115.70	121.00
2	B	185	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	K	229	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	I	229	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	Q	229	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	C	229	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	E	229	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	A	229	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	O	229	ARG	NE-CZ-NH2	8.27	124.44	120.30
1	M	229	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	I	262	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	G	229	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	Q	262	TYR	CB-CG-CD2	-8.21	116.07	121.00
1	A	262	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	C	262	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	M	339	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	G	339	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	O	262	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	E	262	TYR	CB-CG-CD2	-8.11	116.13	121.00
2	D	123	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	E	339	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	K	262	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	K	339	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	I	339	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	G	262	TYR	CB-CG-CD2	-8.08	116.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	262	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	O	339	ARG	NE-CZ-NH2	8.07	124.33	120.30
2	F	123	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	339	ARG	NE-CZ-NH2	8.05	124.32	120.30
2	L	123	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	Q	339	ARG	NE-CZ-NH2	8.02	124.31	120.30
2	H	123	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	R	123	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	11	GLN	CB-CA-C	-8.01	94.38	110.40
2	B	123	ARG	NE-CZ-NH2	-8.01	116.29	120.30
2	N	123	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	C	339	ARG	NE-CZ-NH2	7.98	124.29	120.30
2	J	123	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	K	11	GLN	CB-CA-C	-7.96	94.49	110.40
1	O	11	GLN	CB-CA-C	-7.95	94.50	110.40
1	Q	11	GLN	CB-CA-C	-7.95	94.50	110.40
1	M	11	GLN	CB-CA-C	-7.94	94.51	110.40
1	E	11	GLN	CB-CA-C	-7.94	94.52	110.40
1	A	11	GLN	CB-CA-C	-7.93	94.53	110.40
1	I	11	GLN	CB-CA-C	-7.93	94.53	110.40
1	G	11	GLN	CB-CA-C	-7.93	94.54	110.40
2	P	123	ARG	NE-CZ-NH2	-7.91	116.34	120.30
2	H	311	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	121	ARG	NE-CZ-NH1	-7.85	116.37	120.30
2	P	101	ASN	CB-CG-OD1	-7.83	105.94	121.60
2	L	101	ASN	CB-CG-OD1	-7.82	105.97	121.60
2	J	101	ASN	CB-CG-OD1	-7.81	105.97	121.60
2	N	101	ASN	CB-CG-OD1	-7.80	106.00	121.60
2	H	101	ASN	CB-CG-OD1	-7.80	106.00	121.60
2	F	101	ASN	CB-CG-OD1	-7.79	106.01	121.60
2	B	101	ASN	CB-CG-OD1	-7.79	106.02	121.60
2	R	101	ASN	CB-CG-OD1	-7.79	106.02	121.60
2	N	311	ARG	NE-CZ-NH2	-7.79	116.41	120.30
2	D	101	ASN	CB-CG-OD1	-7.78	106.04	121.60
2	D	311	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	J	311	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	M	121	ARG	NE-CZ-NH1	-7.75	116.42	120.30
2	N	253	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	P	311	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	D	432	TYR	CB-CG-CD2	-7.71	116.37	121.00
2	R	253	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	L	96	GLN	C-N-CA	-7.70	102.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	96	GLN	C-N-CA	-7.70	102.45	121.70
2	N	96	GLN	C-N-CA	-7.70	102.46	121.70
2	L	311	ARG	NE-CZ-NH2	-7.69	116.45	120.30
2	F	400	ARG	NE-CZ-NH1	-7.69	116.46	120.30
2	D	253	ARG	NE-CZ-NH2	7.68	124.14	120.30
2	R	432	TYR	CB-CG-CD2	-7.68	116.39	121.00
2	H	96	GLN	C-N-CA	-7.68	102.51	121.70
2	J	400	ARG	NE-CZ-NH1	-7.68	116.46	120.30
2	D	96	GLN	C-N-CA	-7.67	102.52	121.70
2	L	253	ARG	NE-CZ-NH2	7.67	124.14	120.30
2	P	253	ARG	NE-CZ-NH2	7.67	124.14	120.30
2	N	432	TYR	CB-CG-CD2	-7.66	116.40	121.00
2	P	96	GLN	C-N-CA	-7.66	102.54	121.70
1	Q	121	ARG	NE-CZ-NH1	-7.66	116.47	120.30
2	B	96	GLN	C-N-CA	-7.65	102.57	121.70
2	F	96	GLN	C-N-CA	-7.65	102.58	121.70
2	R	96	GLN	C-N-CA	-7.65	102.57	121.70
2	F	253	ARG	NE-CZ-NH2	7.65	124.12	120.30
2	P	400	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	K	121	ARG	NE-CZ-NH1	-7.64	116.48	120.30
2	L	400	ARG	NE-CZ-NH1	-7.64	116.48	120.30
2	B	253	ARG	NE-CZ-NH2	7.63	124.11	120.30
2	R	311	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	H	400	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	G	121	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	N	400	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	H	432	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	L	432	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	P	432	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	F	311	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	121	ARG	NE-CZ-NH1	-7.61	116.50	120.30
2	B	400	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	B	311	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	I	121	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	F	432	TYR	CB-CG-CD2	-7.57	116.46	121.00
2	B	432	TYR	CB-CG-CD2	-7.56	116.46	121.00
2	F	308	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	E	121	ARG	NE-CZ-NH1	-7.55	116.53	120.30
2	J	308	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	R	400	ARG	NE-CZ-NH1	-7.52	116.54	120.30
2	J	253	ARG	NE-CZ-NH2	7.52	124.06	120.30
2	H	253	ARG	NE-CZ-NH2	7.51	124.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	432	TYR	CB-CG-CD2	-7.50	116.50	121.00
2	D	400	ARG	NE-CZ-NH1	-7.48	116.56	120.30
2	L	308	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	C	185	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	K	185	TYR	CB-CG-CD2	-7.46	116.52	121.00
2	B	308	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	Q	156	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	O	121	ARG	NE-CZ-NH1	-7.44	116.58	120.30
2	R	308	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	G	185	TYR	CB-CG-CD2	-7.43	116.55	121.00
1	O	185	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	O	172	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	I	156	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	172	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	M	172	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	172	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	A	156	ARG	NE-CZ-NH2	7.35	123.98	120.30
2	N	308	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	P	308	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	185	TYR	CB-CG-CD2	-7.34	116.59	121.00
1	M	156	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	I	185	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	C	156	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	E	185	TYR	CB-CG-CD2	-7.31	116.61	121.00
1	M	185	TYR	CB-CG-CD2	-7.31	116.61	121.00
1	G	156	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	G	172	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	E	172	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	Q	185	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	Q	172	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	I	172	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	D	308	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	O	156	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	K	156	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	E	156	ARG	NE-CZ-NH2	7.18	123.89	120.30
2	H	308	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	K	172	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	A	24	TYR	CB-CG-CD1	-7.06	116.76	121.00
1	K	24	TYR	CB-CG-CD1	-7.06	116.76	121.00
1	I	24	TYR	CB-CG-CD1	-7.04	116.77	121.00
1	G	79	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	E	24	TYR	CB-CG-CD1	-7.00	116.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	79	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	O	264	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	C	24	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	Q	24	TYR	CB-CG-CD1	-6.95	116.83	121.00
2	R	320	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	K	264	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	C	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	H	320	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	K	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	M	24	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	A	264	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	G	24	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	I	264	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	O	24	TYR	CB-CG-CD1	-6.90	116.86	121.00
2	N	320	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	E	264	ARG	NE-CZ-NH1	-6.90	116.85	120.30
2	L	320	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	R	2	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	F	2	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	N	2	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	I	79	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	Q	264	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	Q	79	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	79	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	D	2	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	C	264	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	O	79	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	B	320	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	F	320	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	D	320	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	H	2	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	J	320	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	J	2	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	L	2	ARG	NE-CZ-NH2	-6.77	116.91	120.30
2	P	2	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	M	264	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	G	264	ARG	NE-CZ-NH1	-6.76	116.92	120.30
2	B	2	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	P	320	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	E	79	ARG	NE-CZ-NH2	-6.73	116.93	120.30
2	P	79	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	R	79	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	79	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	E	438	ASP	CA-C-N	-6.62	102.63	117.20
1	G	438	ASP	CA-C-N	-6.61	102.66	117.20
1	A	244	PHE	CB-CG-CD2	-6.61	116.17	120.80
2	N	79	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	K	438	ASP	CA-C-N	-6.60	102.68	117.20
1	M	438	ASP	CA-C-N	-6.59	102.69	117.20
2	B	79	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	Q	438	ASP	CA-C-N	-6.59	102.70	117.20
1	O	438	ASP	CA-C-N	-6.59	102.71	117.20
1	G	244	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	E	105	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	438	ASP	CA-C-N	-6.57	102.75	117.20
1	M	105	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	I	438	ASP	CA-C-N	-6.56	102.77	117.20
1	C	438	ASP	CA-C-N	-6.55	102.78	117.20
2	J	79	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	K	244	PHE	CB-CG-CD2	-6.54	116.22	120.80
2	D	79	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	L	79	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	I	244	PHE	CB-CG-CD2	-6.49	116.26	120.80
2	H	79	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	E	244	PHE	CB-CG-CD2	-6.49	116.26	120.80
1	O	244	PHE	CB-CG-CD2	-6.48	116.26	120.80
1	Q	244	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	M	244	PHE	CB-CG-CD2	-6.45	116.28	120.80
1	C	244	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	C	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	K	105	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	105	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	O	105	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	I	105	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	O	142	GLY	C-N-CA	-6.29	109.09	122.30
1	Q	105	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Q	142	GLY	C-N-CA	-6.24	109.19	122.30
1	I	142	GLY	C-N-CA	-6.24	109.20	122.30
1	K	142	GLY	C-N-CA	-6.23	109.21	122.30
1	C	142	GLY	C-N-CA	-6.23	109.21	122.30
1	A	142	GLY	C-N-CA	-6.21	109.26	122.30
1	E	142	GLY	C-N-CA	-6.21	109.27	122.30
1	G	142	GLY	C-N-CA	-6.21	109.27	122.30
1	M	142	GLY	C-N-CA	-6.21	109.27	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	205	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	G	105	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	339	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
1	C	205	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	H	185	TYR	CB-CA-C	-6.13	98.15	110.40
2	L	185	TYR	CB-CA-C	-6.12	98.16	110.40
1	G	339	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
2	J	185	TYR	CB-CA-C	-6.12	98.16	110.40
1	O	11	GLN	N-CA-CB	6.12	121.61	110.60
1	K	190	THR	CB-CA-C	-6.11	95.10	111.60
2	L	306	ASP	CB-CG-OD2	6.11	123.80	118.30
1	G	205	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	I	11	GLN	N-CA-CB	6.11	121.60	110.60
1	I	348	PRO	CA-N-CD	6.11	120.25	111.70
2	R	306	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	11	GLN	N-CA-CB	6.11	121.59	110.60
2	R	185	TYR	CB-CA-C	-6.11	98.18	110.40
2	D	185	TYR	CB-CA-C	-6.11	98.19	110.40
2	F	185	TYR	CB-CA-C	-6.10	98.19	110.40
1	Q	339	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
2	D	306	ASP	CB-CG-OD2	6.10	123.79	118.30
1	M	190	THR	CB-CA-C	-6.10	95.13	111.60
2	B	185	TYR	CB-CA-C	-6.10	98.21	110.40
1	Q	348	PRO	CA-N-CD	6.10	120.23	111.70
1	O	190	THR	CB-CA-C	-6.09	95.15	111.60
1	E	205	ASP	CB-CG-OD2	-6.09	112.82	118.30
2	F	306	ASP	CB-CG-OD2	6.09	123.78	118.30
2	P	185	TYR	CB-CA-C	-6.09	98.22	110.40
1	Q	205	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	11	GLN	N-CA-CB	6.09	121.56	110.60
2	H	306	ASP	CB-CG-OD2	6.09	123.78	118.30
2	J	306	ASP	CB-CG-OD2	6.09	123.78	118.30
1	Q	190	THR	CB-CA-C	-6.08	95.18	111.60
1	C	190	THR	CB-CA-C	-6.08	95.19	111.60
2	N	185	TYR	CB-CA-C	-6.08	98.24	110.40
2	P	306	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	190	THR	CB-CA-C	-6.08	95.20	111.60
1	M	11	GLN	N-CA-CB	6.08	121.54	110.60
1	I	190	THR	CB-CA-C	-6.07	95.20	111.60
1	E	190	THR	CB-CA-C	-6.07	95.20	111.60
1	G	11	GLN	N-CA-CB	6.07	121.53	110.60
1	K	348	PRO	CA-N-CD	6.07	120.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	306	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	348	PRO	CA-N-CD	6.07	120.20	111.70
1	E	11	GLN	N-CA-CB	6.07	121.53	110.60
1	M	205	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	K	11	GLN	N-CA-CB	6.07	121.53	110.60
1	A	348	PRO	CA-N-CD	6.07	120.19	111.70
1	C	339	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	G	190	THR	CB-CA-C	-6.06	95.23	111.60
2	H	311	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	Q	11	GLN	N-CA-CB	6.06	121.51	110.60
1	E	438	ASP	C-N-CA	-6.06	106.56	121.70
2	B	61	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	O	438	ASP	C-N-CA	-6.05	106.57	121.70
2	D	311	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	I	214	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	205	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	G	438	ASP	C-N-CA	-6.04	106.60	121.70
1	M	438	ASP	C-N-CA	-6.04	106.60	121.70
1	O	339	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
1	O	348	PRO	CA-N-CD	6.04	120.15	111.70
1	M	339	ARG	NH1-CZ-NH2	-6.03	112.76	119.40
1	A	339	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	I	339	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	Q	438	ASP	C-N-CA	-6.03	106.63	121.70
1	E	348	PRO	CA-N-CD	6.03	120.13	111.70
1	K	339	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
2	N	306	ASP	CB-CG-OD2	6.03	123.72	118.30
1	C	438	ASP	C-N-CA	-6.02	106.65	121.70
1	I	205	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	H	308	ARG	CD-NE-CZ	6.02	132.02	123.60
1	M	348	PRO	CA-N-CD	6.02	120.12	111.70
2	N	308	ARG	CD-NE-CZ	6.01	132.02	123.60
1	G	348	PRO	CA-N-CD	6.01	120.12	111.70
1	O	205	ASP	CB-CG-OD2	-6.01	112.89	118.30
2	D	61	TYR	CB-CG-CD1	-6.01	117.39	121.00
2	H	61	TYR	CB-CG-CD1	-6.01	117.40	121.00
1	I	438	ASP	C-N-CA	-6.00	106.69	121.70
1	K	438	ASP	C-N-CA	-6.00	106.69	121.70
1	A	438	ASP	C-N-CA	-6.00	106.70	121.70
2	J	311	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	R	308	ARG	CD-NE-CZ	6.00	132.00	123.60
2	D	308	ARG	CD-NE-CZ	5.99	131.98	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	308	ARG	CD-NE-CZ	5.97	131.97	123.60
1	O	108	TYR	CB-CG-CD1	-5.97	117.42	121.00
2	P	308	ARG	CD-NE-CZ	5.97	131.96	123.60
2	J	308	ARG	CD-NE-CZ	5.97	131.95	123.60
2	L	311	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	L	308	ARG	CD-NE-CZ	5.94	131.91	123.60
2	R	253	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
2	R	61	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	P	61	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	G	108	TYR	CB-CG-CD1	-5.92	117.45	121.00
2	F	308	ARG	CD-NE-CZ	5.91	131.87	123.60
2	N	61	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	A	265	GLY	C-N-CA	-5.91	106.94	121.70
2	P	253	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	E	214	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	K	265	GLY	C-N-CA	-5.90	106.95	121.70
1	Q	265	GLY	C-N-CA	-5.90	106.96	121.70
1	G	265	GLY	C-N-CA	-5.89	106.97	121.70
1	M	265	GLY	C-N-CA	-5.89	106.97	121.70
1	I	265	GLY	C-N-CA	-5.89	106.97	121.70
2	L	61	TYR	CB-CG-CD1	-5.89	117.47	121.00
2	R	311	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	I	108	TYR	CB-CG-CD1	-5.88	117.47	121.00
2	J	61	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	M	108	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	E	265	GLY	C-N-CA	-5.87	107.02	121.70
2	J	253	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	C	265	GLY	C-N-CA	-5.87	107.02	121.70
2	N	253	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
1	O	265	GLY	C-N-CA	-5.87	107.03	121.70
2	D	253	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	E	108	TYR	CB-CG-CD1	-5.86	117.48	121.00
2	L	253	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	G	214	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	F	311	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	B	253	ARG	NH1-CZ-NH2	-5.85	112.96	119.40
1	M	214	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	G	438	ASP	O-C-N	5.85	132.05	122.70
2	P	432	TYR	CB-CG-CD1	5.84	124.50	121.00
2	B	311	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	108	TYR	CB-CG-CD1	-5.83	117.50	121.00
2	N	311	ARG	NE-CZ-NH1	5.83	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	61	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	G	11	GLN	CA-CB-CG	5.83	126.22	113.40
2	N	432	TYR	CB-CG-CD1	5.83	124.50	121.00
2	F	253	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	A	108	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	Q	438	ASP	O-C-N	5.82	132.02	122.70
2	B	292	THR	CA-CB-CG2	-5.82	104.25	112.40
2	H	253	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
1	Q	108	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	214	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	E	11	GLN	CA-CB-CG	5.81	126.18	113.40
1	E	438	ASP	O-C-N	5.81	132.00	122.70
2	H	432	TYR	CB-CG-CD1	5.80	124.48	121.00
2	F	292	THR	CA-CB-CG2	-5.80	104.28	112.40
2	J	292	THR	CA-CB-CG2	-5.80	104.28	112.40
1	C	214	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	L	292	THR	CA-CB-CG2	-5.79	104.29	112.40
1	A	11	GLN	CA-CB-CG	5.79	126.14	113.40
1	I	11	GLN	CA-CB-CG	5.79	126.14	113.40
2	R	292	THR	CA-CB-CG2	-5.79	104.29	112.40
2	D	292	THR	CA-CB-CG2	-5.79	104.30	112.40
1	Q	11	GLN	CA-CB-CG	5.79	126.14	113.40
1	M	11	GLN	CA-CB-CG	5.79	126.13	113.40
2	P	292	THR	CA-CB-CG2	-5.79	104.30	112.40
1	C	438	ASP	O-C-N	5.79	131.96	122.70
2	P	311	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	H	248	LEU	CA-C-N	-5.78	104.49	117.20
1	O	438	ASP	O-C-N	5.78	131.94	122.70
1	I	438	ASP	O-C-N	5.78	131.94	122.70
1	K	108	TYR	CB-CG-CD1	-5.78	117.53	121.00
2	F	248	LEU	CA-C-N	-5.77	104.50	117.20
1	O	11	GLN	CA-CB-CG	5.77	126.10	113.40
1	K	11	GLN	CA-CB-CG	5.77	126.10	113.40
2	D	248	LEU	CA-C-N	-5.77	104.51	117.20
1	K	438	ASP	O-C-N	5.77	131.93	122.70
2	N	248	LEU	CA-C-N	-5.77	104.51	117.20
1	C	11	GLN	CA-CB-CG	5.76	126.08	113.40
2	R	248	LEU	CA-C-N	-5.76	104.52	117.20
1	M	438	ASP	O-C-N	5.76	131.92	122.70
2	N	292	THR	CA-CB-CG2	-5.76	104.34	112.40
2	L	248	LEU	CA-C-N	-5.75	104.54	117.20
2	P	248	LEU	CA-C-N	-5.75	104.55	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	432	TYR	CB-CG-CD1	5.75	124.45	121.00
2	D	432	TYR	CB-CG-CD1	5.75	124.45	121.00
2	P	239	THR	CA-CB-CG2	-5.75	104.36	112.40
2	H	292	THR	CA-CB-CG2	-5.74	104.36	112.40
2	H	239	THR	CA-CB-CG2	-5.74	104.36	112.40
1	A	438	ASP	O-C-N	5.74	131.88	122.70
2	B	248	LEU	CA-C-N	-5.73	104.59	117.20
2	J	248	LEU	CA-C-N	-5.73	104.60	117.20
2	F	239	THR	CA-CB-CG2	-5.72	104.39	112.40
2	J	239	THR	CA-CB-CG2	-5.71	104.40	112.40
2	B	239	THR	CA-CB-CG2	-5.71	104.41	112.40
1	Q	214	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	E	236	SER	CB-CA-C	-5.70	99.26	110.10
1	I	236	SER	CB-CA-C	-5.69	99.29	110.10
2	D	239	THR	CA-CB-CG2	-5.69	104.44	112.40
1	G	236	SER	CB-CA-C	-5.68	99.30	110.10
2	L	239	THR	CA-CB-CG2	-5.68	104.44	112.40
1	M	236	SER	CB-CA-C	-5.68	99.31	110.10
1	K	236	SER	CB-CA-C	-5.68	99.31	110.10
1	Q	236	SER	CB-CA-C	-5.68	99.31	110.10
2	R	239	THR	CA-CB-CG2	-5.67	104.46	112.40
1	A	236	SER	CB-CA-C	-5.67	99.32	110.10
2	N	239	THR	CA-CB-CG2	-5.67	104.46	112.40
2	F	432	TYR	CB-CG-CD1	5.66	124.40	121.00
1	O	236	SER	CB-CA-C	-5.66	99.35	110.10
1	K	306	ASP	CB-CG-OD1	5.64	123.38	118.30
2	B	432	TYR	CB-CG-CD1	5.64	124.38	121.00
1	O	214	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	236	SER	CB-CA-C	-5.63	99.41	110.10
2	L	432	TYR	CB-CG-CD1	5.63	124.38	121.00
1	O	306	ASP	CB-CG-OD1	5.62	123.36	118.30
2	B	101	ASN	CA-CB-CG	-5.61	101.06	113.40
1	G	306	ASP	CB-CG-OD1	5.61	123.35	118.30
2	J	101	ASN	CA-CB-CG	-5.61	101.06	113.40
2	D	101	ASN	CA-CB-CG	-5.61	101.07	113.40
2	F	101	ASN	CB-CG-ND2	5.61	130.15	116.70
2	P	101	ASN	CA-CB-CG	-5.60	101.08	113.40
2	L	101	ASN	CA-CB-CG	-5.60	101.08	113.40
2	H	101	ASN	CB-CG-ND2	5.60	130.13	116.70
2	N	101	ASN	CA-CB-CG	-5.59	101.09	113.40
2	R	101	ASN	CA-CB-CG	-5.59	101.10	113.40
2	P	101	ASN	CB-CG-ND2	5.59	130.12	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	101	ASN	CA-CB-CG	-5.59	101.11	113.40
2	D	101	ASN	CB-CG-ND2	5.58	130.09	116.70
2	J	101	ASN	CB-CG-ND2	5.58	130.09	116.70
1	K	214	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	R	101	ASN	CB-CG-ND2	5.58	130.08	116.70
1	I	306	ASP	CB-CG-OD1	5.57	123.31	118.30
2	L	101	ASN	CB-CG-ND2	5.57	130.07	116.70
1	C	161	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	M	121	ARG	NE-CZ-NH2	5.57	123.08	120.30
2	N	101	ASN	CB-CG-ND2	5.56	130.05	116.70
2	H	101	ASN	CA-CB-CG	-5.56	101.17	113.40
2	B	101	ASN	CB-CG-ND2	5.56	130.03	116.70
1	C	123	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	J	432	TYR	CB-CG-CD1	5.55	124.33	121.00
1	A	121	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	F	215	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	F	401	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	C	306	ASP	CB-CG-OD1	5.52	123.27	118.30
1	Q	161	TYR	CB-CG-CD1	-5.50	117.70	121.00
2	H	401	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
2	L	401	ARG	NH1-CZ-NH2	-5.49	113.37	119.40
1	E	161	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	161	TYR	CB-CG-CD1	-5.48	117.71	121.00
2	D	401	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	E	306	ASP	CB-CG-OD1	5.48	123.23	118.30
2	J	401	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	M	306	ASP	CB-CG-OD1	5.48	123.23	118.30
2	R	401	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	Q	306	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	306	ASP	CB-CG-OD1	5.46	123.22	118.30
2	J	48	ARG	CD-NE-CZ	5.46	131.25	123.60
1	I	161	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	N	48	ARG	CD-NE-CZ	5.46	131.24	123.60
2	D	48	ARG	CD-NE-CZ	5.45	131.23	123.60
1	I	211	ASP	CB-CG-OD2	5.45	123.20	118.30
2	L	48	ARG	CD-NE-CZ	5.44	131.22	123.60
1	Q	211	ASP	CB-CG-OD2	5.44	123.19	118.30
2	N	401	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
2	F	48	ARG	CD-NE-CZ	5.43	131.20	123.60
2	B	48	ARG	CD-NE-CZ	5.43	131.20	123.60
1	G	161	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	E	339	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	48	ARG	CD-NE-CZ	5.42	131.19	123.60
2	P	401	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
2	B	401	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
1	A	211	ASP	CB-CG-OD2	5.42	123.18	118.30
2	P	48	ARG	CD-NE-CZ	5.42	131.18	123.60
2	P	53	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	M	123	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	O	123	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	J	253	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	O	161	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	Q	339	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	211	ASP	CB-CG-OD2	5.40	123.16	118.30
1	K	211	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	211	ASP	CB-CG-OD2	5.39	123.15	118.30
1	O	211	ASP	CB-CG-OD2	5.39	123.16	118.30
2	R	48	ARG	CD-NE-CZ	5.39	131.15	123.60
2	R	53	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	E	123	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	G	211	ASP	CB-CG-OD2	5.39	123.15	118.30
1	K	161	TYR	CB-CG-CD1	-5.39	117.77	121.00
2	H	53	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	K	123	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	M	211	ASP	CB-CG-OD2	5.38	123.14	118.30
1	Q	123	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	F	97	SER	CA-C-N	-5.38	105.45	116.20
2	N	215	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	J	97	SER	CA-C-N	-5.37	105.45	116.20
2	H	97	SER	CA-C-N	-5.36	105.48	116.20
2	N	97	SER	CA-C-N	-5.36	105.48	116.20
2	B	185	TYR	CA-CB-CG	5.36	123.58	113.40
2	P	97	SER	CA-C-N	-5.36	105.48	116.20
2	L	53	TYR	CB-CG-CD2	-5.36	117.79	121.00
2	F	53	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	339	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	Q	121	ARG	NE-CZ-NH2	5.35	122.98	120.30
2	D	53	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	J	185	TYR	CA-CB-CG	5.35	123.56	113.40
2	L	97	SER	CA-C-N	-5.35	105.50	116.20
2	D	97	SER	CA-C-N	-5.35	105.51	116.20
2	R	97	SER	CA-C-N	-5.35	105.51	116.20
2	P	185	TYR	CA-CB-CG	5.34	123.56	113.40
2	N	185	TYR	CA-CB-CG	5.34	123.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	161	TYR	CB-CG-CD1	-5.34	117.80	121.00
2	B	97	SER	CA-C-N	-5.34	105.52	116.20
2	J	53	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	R	253	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	D	185	TYR	CA-CB-CG	5.32	123.51	113.40
1	G	339	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	P	253	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	K	121	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	D	61	TYR	CA-CB-CG	-5.31	103.31	113.40
2	H	61	TYR	CA-CB-CG	-5.31	103.32	113.40
2	R	185	TYR	CA-CB-CG	5.31	123.48	113.40
2	N	61	TYR	CA-CB-CG	-5.30	103.32	113.40
2	F	185	TYR	CA-CB-CG	5.30	123.47	113.40
2	B	61	TYR	CA-CB-CG	-5.29	103.34	113.40
2	F	61	TYR	CA-CB-CG	-5.29	103.34	113.40
1	I	121	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	R	215	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	B	53	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	H	253	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	R	61	TYR	CA-CB-CG	-5.28	103.37	113.40
2	H	185	TYR	CA-CB-CG	5.28	123.43	113.40
2	D	215	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	J	61	TYR	CA-CB-CG	-5.27	103.39	113.40
1	I	123	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	L	185	TYR	CA-CB-CG	5.27	123.41	113.40
2	L	61	TYR	CA-CB-CG	-5.27	103.39	113.40
2	J	215	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	P	61	TYR	CA-CB-CG	-5.26	103.41	113.40
2	N	53	TYR	CB-CG-CD2	-5.26	117.85	121.00
2	P	215	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	123	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	G	123	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	253	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	L	215	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	98	ASP	CA-C-N	-5.23	105.69	117.20
1	M	98	ASP	CA-C-N	-5.23	105.68	117.20
1	C	121	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	E	121	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	G	121	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	K	98	ASP	CA-C-N	-5.22	105.71	117.20
1	A	339	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	L	253	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	ASP	CA-C-N	-5.21	105.73	117.20
2	D	253	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	H	161	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	O	339	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	Q	98	ASP	CA-C-N	-5.21	105.75	117.20
1	O	98	ASP	CA-C-N	-5.20	105.76	117.20
2	D	306	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	G	98	ASP	CA-C-N	-5.19	105.78	117.20
1	I	98	ASP	CA-C-N	-5.19	105.78	117.20
1	K	347	CYS	N-CA-C	5.19	125.00	111.00
1	O	347	CYS	N-CA-C	5.19	125.00	111.00
1	E	98	ASP	CA-C-N	-5.18	105.80	117.20
2	L	306	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	N	253	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	347	CYS	N-CA-C	5.18	124.97	111.00
1	I	347	CYS	N-CA-C	5.18	124.98	111.00
1	E	347	CYS	N-CA-C	5.17	124.97	111.00
1	I	339	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	F	253	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	347	CYS	N-CA-C	5.17	124.94	111.00
2	F	306	ASP	CB-CG-OD1	-5.16	113.65	118.30
1	Q	347	CYS	N-CA-C	5.16	124.94	111.00
1	A	347	CYS	N-CA-C	5.16	124.94	111.00
1	K	339	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	P	306	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	M	347	CYS	N-CA-C	5.16	124.92	111.00
2	R	306	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	L	435	TYR	CB-CG-CD2	-5.14	117.92	121.00
2	J	306	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	M	339	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	R	161	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	B	215	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	O	121	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	F	435	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	N	435	TYR	CB-CG-CD2	-5.09	117.94	121.00
2	R	435	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	B	306	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	N	306	ASP	CB-CG-OD1	-5.08	113.73	118.30
2	B	435	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	P	161	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	G	312	TYR	CB-CG-CD2	-5.04	117.98	121.00
2	H	435	TYR	CB-CG-CD2	-5.03	117.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	161	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	H	185	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	312	TYR	CB-CG-CD2	-5.01	117.99	121.00
2	R	96	GLN	N-CA-C	5.00	124.51	111.00
2	H	306	ASP	CB-CG-OD1	-5.00	113.80	118.30
2	L	161	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LEU	Peptide
2	D	248	LEU	Peptide
2	F	248	LEU	Peptide
2	H	248	LEU	Peptide
2	J	248	LEU	Peptide
2	L	248	LEU	Peptide
2	N	248	LEU	Peptide
2	P	248	LEU	Peptide
2	R	248	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	399	0
1	C	3350	0	3254	363	0
1	E	3350	0	3254	369	0
1	G	3350	0	3254	372	0
1	I	3350	0	3254	391	0
1	K	3350	0	3254	369	0
1	M	3350	0	3254	302	0
1	O	3350	0	3254	332	0
1	Q	3350	0	3254	300	0
2	B	3352	0	3227	391	0
2	D	3352	0	3227	358	0
2	F	3352	0	3227	358	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	3352	0	3227	301	0
2	J	3352	0	3227	329	0
2	L	3352	0	3227	302	0
2	N	3352	0	3227	408	0
2	P	3352	0	3227	467	0
2	R	3352	0	3227	405	0
3	A	32	0	12	3	0
3	C	32	0	12	3	0
3	E	32	0	12	3	0
3	G	32	0	12	3	0
3	I	32	0	12	3	0
3	K	32	0	12	3	0
3	M	32	0	12	3	0
3	O	32	0	12	3	0
3	Q	32	0	12	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0
5	P	28	0	12	3	0
5	R	28	0	12	2	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
6	E	4	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	K	4	0	0	0	0
6	M	4	0	0	0	0
6	O	4	0	0	0	0
6	Q	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	60903	0	58545	3577	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (3577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:CA	2:H:352:LYS:HE3	1.19	1.64
1:E:181:VAL:CA	2:F:352:LYS:HE3	1.25	1.62
1:I:181:VAL:CA	2:J:352:LYS:HE3	1.17	1.61
1:C:181:VAL:CA	2:D:352:LYS:HE3	1.28	1.58
1:M:181:VAL:CA	2:N:352:LYS:HE3	1.17	1.58
1:K:181:VAL:CA	2:L:352:LYS:HE3	1.18	1.58
1:A:181:VAL:CA	2:B:352:LYS:HE3	1.28	1.57
1:O:181:VAL:CA	2:P:352:LYS:HE3	1.11	1.57
1:Q:181:VAL:CA	2:R:352:LYS:HE3	1.16	1.55
1:O:181:VAL:HA	2:P:352:LYS:CE	1.38	1.52
1:I:224:TYR:CE1	2:J:325:MET:SD	2.04	1.51
1:K:224:TYR:CE1	2:L:325:MET:SD	2.04	1.50
1:O:101:ASN:CB	2:P:254:LYS:HE3	1.33	1.50
1:O:176:GLN:CB	2:P:333:LEU:HD22	1.37	1.48
1:I:101:ASN:CB	2:J:254:LYS:HE3	1.40	1.48
1:O:176:GLN:HB3	2:P:333:LEU:CD2	1.43	1.47
1:G:224:TYR:CE1	2:H:325:MET:SD	2.08	1.47
1:Q:101:ASN:CB	2:R:254:LYS:HE3	1.43	1.47
1:M:101:ASN:CB	2:N:254:LYS:HE3	1.40	1.47
1:G:101:ASN:CB	2:H:254:LYS:HE3	1.43	1.46
1:M:176:GLN:CB	2:N:333:LEU:HD22	1.44	1.46
1:M:181:VAL:HA	2:N:352:LYS:CE	1.44	1.45
1:K:101:ASN:CB	2:L:254:LYS:HE3	1.45	1.45
1:O:210:TYR:CE2	2:P:326:LYS:HA	1.53	1.44
1:Q:181:VAL:HA	2:R:352:LYS:CE	1.44	1.44
1:I:176:GLN:HB3	2:J:333:LEU:CD2	1.48	1.44
1:A:346:TRP:CZ3	2:P:403:ALA:HB1	1.52	1.43
1:A:346:TRP:CE3	2:P:403:ALA:HB2	1.53	1.43
1:I:176:GLN:CB	2:J:333:LEU:HD22	1.45	1.43
1:Q:176:GLN:CB	2:R:333:LEU:HD22	1.44	1.42
1:G:176:GLN:CB	2:H:333:LEU:HD22	1.48	1.42
1:A:101:ASN:CB	2:B:254:LYS:HE3	1.49	1.42
1:O:179:THR:CG2	2:P:353:THR:OG1	1.68	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:GLN:HB3	2:N:333:LEU:CD2	1.49	1.42
1:Q:176:GLN:HB3	2:R:333:LEU:CD2	1.47	1.42
1:I:181:VAL:HA	2:J:352:LYS:CE	1.48	1.42
1:A:2:ARG:CG	2:P:96:GLN:HE22	1.30	1.41
1:G:176:GLN:HB3	2:H:333:LEU:CD2	1.50	1.41
1:O:101:ASN:HB2	2:P:254:LYS:CE	1.46	1.41
1:E:224:TYR:CE1	2:F:325:MET:SD	2.14	1.41
1:K:176:GLN:CB	2:L:333:LEU:HD22	1.49	1.41
1:E:346:TRP:CZ3	2:R:403:ALA:HB1	1.55	1.40
1:I:101:ASN:HB2	2:J:254:LYS:CE	1.49	1.40
1:K:176:GLN:HB3	2:L:333:LEU:CD2	1.48	1.40
1:A:224:TYR:CE1	2:B:325:MET:SD	2.13	1.40
1:C:101:ASN:CB	2:D:254:LYS:HE3	1.51	1.40
1:M:210:TYR:CE2	2:N:326:LYS:HA	1.57	1.40
1:A:329:ASN:OD1	2:P:177:VAL:CG2	1.67	1.39
1:A:346:TRP:HB3	2:P:401:ARG:CG	1.50	1.39
1:C:224:TYR:CE1	2:D:325:MET:SD	2.16	1.39
1:C:346:TRP:CZ3	2:N:403:ALA:HB1	1.57	1.38
1:G:181:VAL:HA	2:H:352:LYS:CE	1.51	1.38
1:I:210:TYR:CE2	2:J:326:LYS:HA	1.59	1.38
1:C:2:ARG:CG	2:N:96:GLN:HE22	1.36	1.37
1:G:101:ASN:HB2	2:H:254:LYS:CE	1.52	1.37
1:K:181:VAL:HA	2:L:352:LYS:CE	1.51	1.37
1:Q:210:TYR:CZ	2:R:326:LYS:HA	1.60	1.37
1:Q:210:TYR:CE2	2:R:326:LYS:HA	1.59	1.37
1:E:346:TRP:CE3	2:R:403:ALA:HB2	1.59	1.36
1:A:2:ARG:HG3	2:P:96:GLN:NE2	1.36	1.36
1:K:101:ASN:HB2	2:L:254:LYS:CE	1.55	1.36
1:E:101:ASN:CB	2:F:254:LYS:HE3	1.54	1.36
1:C:346:TRP:CE3	2:N:403:ALA:HB2	1.59	1.36
1:M:101:ASN:HB2	2:N:254:LYS:CE	1.52	1.36
1:O:210:TYR:CE1	2:P:326:LYS:HB2	1.58	1.36
1:Q:101:ASN:HB2	2:R:254:LYS:CE	1.55	1.36
1:M:179:THR:HG22	2:N:353:THR:OG1	1.18	1.35
1:C:2:ARG:HG3	2:N:96:GLN:NE2	1.41	1.35
1:M:179:THR:CG2	2:N:353:THR:OG1	1.73	1.35
1:Q:210:TYR:CE1	2:R:326:LYS:HB2	1.60	1.35
1:C:346:TRP:HB3	2:N:401:ARG:CG	1.56	1.34
1:E:329:ASN:OD1	2:R:177:VAL:CG2	1.72	1.34
1:Q:179:THR:CG2	2:R:353:THR:OG1	1.74	1.34
1:C:329:ASN:OD1	2:N:177:VAL:CG2	1.72	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:210:TYR:CZ	2:P:326:LYS:HA	1.61	1.34
2:B:403:ALA:HB1	1:I:346:TRP:CZ3	1.61	1.34
1:G:210:TYR:CE2	2:H:326:LYS:HA	1.62	1.34
1:A:346:TRP:CB	2:P:401:ARG:HG3	1.56	1.34
1:A:350:GLY:O	2:P:181:VAL:CG2	1.77	1.33
1:E:2:ARG:CG	2:R:96:GLN:HE22	1.39	1.33
1:M:210:TYR:CZ	2:N:326:LYS:HA	1.62	1.33
1:A:346:TRP:CZ3	2:P:403:ALA:CB	2.11	1.33
1:A:101:ASN:HB2	2:B:254:LYS:CE	1.57	1.33
1:A:181:VAL:HA	2:B:352:LYS:CE	1.58	1.32
1:M:210:TYR:CE1	2:N:326:LYS:HB2	1.62	1.32
2:D:177:VAL:HG23	1:G:329:ASN:OD1	1.14	1.32
1:E:181:VAL:HA	2:F:352:LYS:CE	1.58	1.32
2:F:177:VAL:HG23	1:K:329:ASN:OD1	1.16	1.31
1:K:210:TYR:CE2	2:L:326:LYS:HA	1.65	1.31
1:O:210:TYR:CZ	2:P:326:LYS:CA	2.13	1.31
1:I:179:THR:CG2	2:J:353:THR:OG1	1.79	1.31
1:K:210:TYR:CZ	2:L:326:LYS:HA	1.66	1.31
1:C:181:VAL:HA	2:D:352:LYS:CE	1.59	1.31
1:I:210:TYR:CE1	2:J:326:LYS:HB2	1.62	1.31
2:J:283:TYR:HA	2:L:56:ALA:CB	1.57	1.31
1:C:350:GLY:O	2:N:181:VAL:HG22	1.23	1.31
1:G:179:THR:HG22	2:H:353:THR:OG1	1.25	1.31
1:Q:97:GLU:CD	2:R:2:ARG:HH21	1.34	1.31
2:D:403:ALA:HB1	1:G:346:TRP:CZ3	1.66	1.30
1:O:97:GLU:OE2	2:P:2:ARG:NE	1.61	1.30
1:C:101:ASN:HB2	2:D:254:LYS:CE	1.60	1.30
1:O:97:GLU:CD	2:P:2:ARG:HH21	1.35	1.30
1:O:101:ASN:N	2:P:254:LYS:HD2	1.45	1.30
2:B:403:ALA:HB2	1:I:346:TRP:CE3	1.65	1.30
1:C:346:TRP:CB	2:N:401:ARG:HG3	1.59	1.30
1:C:176:GLN:CB	2:D:333:LEU:HD22	1.61	1.29
1:E:176:GLN:HB3	2:F:333:LEU:CD2	1.59	1.29
1:I:210:TYR:CZ	2:J:326:LYS:HA	1.66	1.29
1:K:210:TYR:CE1	2:L:326:LYS:HB2	1.64	1.29
1:O:97:GLU:OE1	2:P:2:ARG:NH2	1.63	1.29
2:P:283:TYR:HA	2:R:56:ALA:CB	1.61	1.29
1:G:210:TYR:CE1	2:H:326:LYS:HB2	1.66	1.29
2:B:177:VAL:CG2	1:I:329:ASN:OD1	1.78	1.29
1:O:179:THR:HG22	2:P:353:THR:OG1	1.12	1.29
1:E:346:TRP:HB3	2:R:401:ARG:CG	1.62	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:210:TYR:CZ	2:R:326:LYS:CA	2.16	1.28
1:A:176:GLN:CB	2:B:333:LEU:HD22	1.61	1.28
1:A:179:THR:HG22	2:B:353:THR:OG1	1.28	1.28
1:E:176:GLN:CB	2:F:333:LEU:HD22	1.62	1.28
1:I:97:GLU:OE2	2:J:2:ARG:NE	1.66	1.28
1:C:176:GLN:HB3	2:D:333:LEU:CD2	1.62	1.28
1:C:346:TRP:CZ3	2:N:403:ALA:CB	2.16	1.28
2:F:403:ALA:HB1	1:K:346:TRP:CZ3	1.67	1.28
1:I:179:THR:HG22	2:J:353:THR:OG1	1.22	1.28
1:M:210:TYR:CZ	2:N:326:LYS:CA	2.17	1.28
1:A:176:GLN:HB3	2:B:333:LEU:CD2	1.63	1.27
1:M:97:GLU:CD	2:N:2:ARG:HH21	1.36	1.27
1:O:210:TYR:CD1	2:P:326:LYS:HB2	1.69	1.27
2:B:177:VAL:HG23	1:I:329:ASN:OD1	1.09	1.27
1:E:101:ASN:HB2	2:F:254:LYS:CE	1.64	1.27
1:E:2:ARG:HG3	2:R:96:GLN:NE2	1.47	1.27
1:A:350:GLY:O	2:P:181:VAL:HG22	1.18	1.26
2:B:401:ARG:CG	1:I:346:TRP:HB3	1.65	1.26
1:E:346:TRP:CZ3	2:R:403:ALA:CB	2.17	1.26
2:B:181:VAL:HG22	1:I:350:GLY:O	1.31	1.26
1:C:350:GLY:O	2:N:181:VAL:CG2	1.83	1.26
1:E:350:GLY:O	2:R:181:VAL:HG22	1.30	1.26
1:G:179:THR:CG2	2:H:353:THR:OG1	1.83	1.26
2:D:177:VAL:CG2	1:G:329:ASN:OD1	1.82	1.26
1:K:179:THR:CG2	2:L:353:THR:OG1	1.83	1.26
1:A:210:TYR:CE2	2:B:326:LYS:HA	1.71	1.26
2:D:96:GLN:HE22	1:G:2:ARG:CG	1.49	1.26
1:K:97:GLU:CD	2:L:2:ARG:HH21	1.39	1.26
1:O:177:VAL:HG21	2:P:329:ASP:C	1.53	1.25
1:M:97:GLU:OE2	2:N:2:ARG:NE	1.67	1.25
1:M:210:TYR:CD1	2:N:326:LYS:HB2	1.72	1.25
1:Q:177:VAL:HG21	2:R:329:ASP:O	1.36	1.25
1:Q:179:THR:HG22	2:R:353:THR:OG1	1.22	1.25
2:B:96:GLN:HE22	1:I:2:ARG:CG	1.49	1.25
1:C:179:THR:HG22	2:D:353:THR:OG1	1.30	1.25
1:I:210:TYR:CZ	2:J:326:LYS:CA	2.20	1.25
1:A:260:VAL:O	2:P:406:HIS:CE1	1.87	1.25
1:E:97:GLU:CD	2:F:2:ARG:HH21	1.39	1.25
2:D:96:GLN:NE2	1:G:2:ARG:HG3	1.52	1.24
1:G:210:TYR:CZ	2:H:326:LYS:HA	1.70	1.24
2:H:283:TYR:HA	2:J:56:ALA:CB	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:210:TYR:CD1	2:R:326:LYS:HB2	1.72	1.24
1:O:105:ARG:NH2	2:P:253:ARG:NH2	1.84	1.24
2:D:403:ALA:HB2	1:G:346:TRP:CE3	1.70	1.24
2:F:177:VAL:CG2	1:K:329:ASN:OD1	1.83	1.24
1:I:97:GLU:CD	2:J:2:ARG:HH21	1.41	1.24
1:K:179:THR:HG22	2:L:353:THR:OG1	1.29	1.24
1:O:177:VAL:HG21	2:P:329:ASP:O	1.34	1.24
1:G:97:GLU:OE2	2:H:2:ARG:NE	1.70	1.24
1:M:97:GLU:OE1	2:N:2:ARG:NH2	1.69	1.24
1:M:101:ASN:N	2:N:254:LYS:HD2	1.50	1.24
1:Q:97:GLU:OE2	2:R:2:ARG:NE	1.69	1.24
2:F:403:ALA:HB2	1:K:346:TRP:CE3	1.72	1.23
1:A:179:THR:CG2	2:B:353:THR:OG1	1.86	1.23
2:B:401:ARG:HG3	1:I:346:TRP:CB	1.67	1.23
1:C:210:TYR:CE2	2:D:326:LYS:HA	1.72	1.23
1:E:346:TRP:CB	2:R:401:ARG:HG3	1.67	1.23
1:K:210:TYR:CZ	2:L:326:LYS:CA	2.22	1.23
1:E:179:THR:HG22	2:F:353:THR:OG1	1.36	1.23
1:K:97:GLU:OE2	2:L:2:ARG:NE	1.69	1.23
2:B:96:GLN:NE2	1:I:2:ARG:HG3	1.53	1.22
2:B:403:ALA:CB	1:I:346:TRP:CZ3	2.23	1.22
1:A:97:GLU:CD	2:B:2:ARG:HH21	1.42	1.22
1:M:76:ASP:OD2	2:N:48:ARG:NH2	1.71	1.22
1:I:210:TYR:CD1	2:J:326:LYS:HB2	1.74	1.22
1:Q:101:ASN:N	2:R:254:LYS:HD2	1.53	1.22
1:A:97:GLU:OE2	2:B:2:ARG:NE	1.73	1.21
1:E:350:GLY:O	2:R:181:VAL:CG2	1.88	1.21
2:F:96:GLN:HE22	1:K:2:ARG:CG	1.52	1.21
2:N:283:TYR:HA	2:P:56:ALA:CB	1.68	1.21
2:D:401:ARG:CG	1:G:346:TRP:HB3	1.70	1.21
1:E:210:TYR:CE2	2:F:326:LYS:HA	1.76	1.21
1:E:329:ASN:OD1	2:R:177:VAL:HG23	1.05	1.21
1:Q:97:GLU:OE1	2:R:2:ARG:NH2	1.71	1.21
1:O:177:VAL:CG2	2:P:329:ASP:O	1.88	1.21
2:D:181:VAL:HG22	1:G:350:GLY:O	1.34	1.21
1:G:210:TYR:CZ	2:H:326:LYS:CA	2.24	1.21
1:M:177:VAL:HG21	2:N:329:ASP:O	1.38	1.21
1:A:210:TYR:CZ	2:B:326:LYS:HA	1.76	1.20
1:M:222:PRO:O	2:N:324:SER:HB2	1.41	1.20
1:C:97:GLU:CD	2:D:2:ARG:HH21	1.44	1.20
1:C:179:THR:CG2	2:D:353:THR:OG1	1.89	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:ARG:NH2	2:N:253:ARG:NH2	1.90	1.20
2:D:401:ARG:HG3	1:G:346:TRP:CB	1.69	1.20
1:E:76:ASP:OD2	2:F:48:ARG:NH2	1.75	1.20
1:G:97:GLU:CD	2:H:2:ARG:HH21	1.43	1.20
1:Q:76:ASP:OD2	2:R:48:ARG:NH2	1.71	1.20
1:Q:222:PRO:O	2:R:324:SER:HB2	1.40	1.20
1:M:177:VAL:HG21	2:N:329:ASP:C	1.60	1.20
1:C:260:VAL:O	2:N:406:HIS:CE1	1.94	1.20
2:F:181:VAL:HG22	1:K:350:GLY:O	1.38	1.20
1:I:101:ASN:N	2:J:254:LYS:HD2	1.57	1.20
1:A:76:ASP:OD2	2:B:48:ARG:NH2	1.75	1.19
1:C:329:ASN:OD1	2:N:177:VAL:HG23	1.02	1.19
1:E:210:TYR:CZ	2:F:326:LYS:HA	1.77	1.19
1:O:222:PRO:O	2:P:324:SER:HB2	1.39	1.19
1:I:97:GLU:OE1	2:J:2:ARG:NH2	1.74	1.19
1:G:210:TYR:CD1	2:H:326:LYS:HB2	1.78	1.19
2:F:96:GLN:NE2	1:K:2:ARG:HG3	1.57	1.19
1:O:76:ASP:OD2	2:P:48:ARG:NH2	1.72	1.19
1:K:181:VAL:CA	2:L:352:LYS:CE	2.13	1.19
1:C:210:TYR:CZ	2:D:326:LYS:HA	1.78	1.18
1:O:406:HIS:CE1	2:P:260:VAL:HG12	1.76	1.18
2:F:401:ARG:CG	1:K:346:TRP:HB3	1.74	1.18
1:Q:177:VAL:HG21	2:R:329:ASP:C	1.62	1.18
1:E:179:THR:CG2	2:F:353:THR:OG1	1.91	1.18
1:O:97:GLU:CD	2:P:2:ARG:NH2	1.96	1.18
1:Q:97:GLU:CD	2:R:2:ARG:NH2	1.97	1.18
1:A:210:TYR:CE1	2:B:326:LYS:HB2	1.78	1.17
2:B:181:VAL:CG2	1:I:350:GLY:O	1.92	1.17
1:K:210:TYR:CD1	2:L:326:LYS:HB2	1.78	1.17
1:I:76:ASP:OD2	2:J:48:ARG:NH2	1.76	1.17
1:A:353:VAL:HB	2:P:179:ASP:OD1	1.42	1.17
2:D:403:ALA:CB	1:G:346:TRP:CZ3	2.27	1.17
1:O:404:PHE:N	2:P:261:PRO:HA	1.58	1.17
1:A:260:VAL:O	2:P:406:HIS:HE1	1.19	1.17
1:E:210:TYR:CE1	2:F:326:LYS:HB2	1.78	1.17
2:F:401:ARG:HG3	1:K:346:TRP:CB	1.74	1.17
1:G:181:VAL:CA	2:H:352:LYS:CE	2.15	1.17
1:I:177:VAL:HG21	2:J:329:ASP:C	1.61	1.17
1:I:181:VAL:CA	2:J:352:LYS:CE	2.13	1.17
1:I:222:PRO:O	2:J:324:SER:HB2	1.43	1.17
1:C:97:GLU:OE2	2:D:2:ARG:NE	1.78	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ALA:HA	2:F:254:LYS:HB2	1.27	1.16
1:K:177:VAL:HG21	2:L:329:ASP:O	1.45	1.16
1:M:97:GLU:CD	2:N:2:ARG:NH2	1.99	1.16
1:C:260:VAL:O	2:N:406:HIS:HE1	1.23	1.16
1:C:210:TYR:CE1	2:D:326:LYS:HB2	1.80	1.16
1:G:177:VAL:HG21	2:H:329:ASP:C	1.64	1.16
1:K:97:GLU:OE1	2:L:2:ARG:NH2	1.77	1.16
1:E:181:VAL:CA	2:F:352:LYS:CE	2.20	1.16
1:E:346:TRP:CE3	2:R:403:ALA:CB	2.28	1.16
1:G:101:ASN:N	2:H:254:LYS:HD2	1.61	1.16
1:K:76:ASP:OD2	2:L:48:ARG:NH2	1.75	1.16
1:Q:105:ARG:NH2	2:R:253:ARG:NH2	1.93	1.16
1:C:76:ASP:OD2	2:D:48:ARG:NH2	1.77	1.15
1:E:260:VAL:O	2:R:406:HIS:CE1	1.98	1.15
1:M:406:HIS:CE1	2:N:260:VAL:HG12	1.80	1.15
1:A:97:GLU:OE1	2:B:2:ARG:NH2	1.78	1.15
1:A:100:ALA:HA	2:B:254:LYS:HB2	1.25	1.15
1:A:346:TRP:CE3	2:P:403:ALA:CB	2.27	1.15
1:A:133:GLN:NE2	2:P:97:SER:OG	1.80	1.15
1:E:260:VAL:O	2:R:406:HIS:HE1	1.28	1.15
1:I:177:VAL:HG21	2:J:329:ASP:O	1.43	1.15
1:O:105:ARG:HH21	2:P:253:ARG:NH2	1.42	1.15
1:O:176:GLN:OE1	2:P:333:LEU:HD11	1.44	1.15
1:Q:100:ALA:HA	2:R:254:LYS:HB2	1.16	1.15
1:G:76:ASP:OD2	2:H:48:ARG:NH2	1.78	1.15
1:G:222:PRO:O	2:H:324:SER:HB2	1.46	1.15
1:M:100:ALA:HA	2:N:254:LYS:HB2	1.15	1.15
1:G:97:GLU:OE1	2:H:2:ARG:NH2	1.79	1.14
2:J:283:TYR:CA	2:L:56:ALA:CB	2.24	1.14
1:K:101:ASN:N	2:L:254:LYS:HD2	1.62	1.14
1:I:100:ALA:HA	2:J:254:LYS:HB2	1.26	1.14
1:K:222:PRO:O	2:L:324:SER:HB2	1.46	1.14
1:M:177:VAL:CG2	2:N:329:ASP:O	1.94	1.14
1:C:100:ALA:HA	2:D:254:LYS:HB2	1.27	1.14
1:K:97:GLU:CD	2:L:2:ARG:NH2	2.00	1.14
1:K:177:VAL:HG21	2:L:329:ASP:C	1.67	1.14
1:M:404:PHE:N	2:N:261:PRO:HA	1.63	1.14
1:Q:177:VAL:CG2	2:R:329:ASP:O	1.94	1.14
2:F:403:ALA:CB	1:K:346:TRP:CZ3	2.30	1.14
1:A:101:ASN:N	2:B:254:LYS:HD2	1.61	1.13
1:I:404:PHE:H	2:J:261:PRO:HA	1.10	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:406:HIS:CE1	2:R:260:VAL:HG12	1.82	1.13
1:A:329:ASN:OD1	2:P:177:VAL:HG23	0.96	1.13
2:P:283:TYR:CA	2:R:56:ALA:CB	2.25	1.13
1:G:177:VAL:HG21	2:H:329:ASP:O	1.47	1.13
1:I:97:GLU:CD	2:J:2:ARG:NH2	2.01	1.13
1:O:100:ALA:HA	2:P:254:LYS:HB2	1.14	1.13
3:Q:501:GTP:O3G	2:R:254:LYS:NZ	1.80	1.13
2:D:181:VAL:CG2	1:G:350:GLY:O	1.97	1.12
1:K:100:ALA:HA	2:L:254:LYS:HB2	1.26	1.12
1:M:176:GLN:OE1	2:N:333:LEU:HD11	1.48	1.12
1:M:105:ARG:HH21	2:N:253:ARG:NH2	1.46	1.12
1:C:353:VAL:HB	2:N:179:ASP:OD1	1.46	1.12
1:G:100:ALA:HA	2:H:254:LYS:HB2	1.28	1.12
2:H:283:TYR:HD2	2:J:62:VAL:HG22	1.11	1.12
1:O:210:TYR:CD2	2:P:326:LYS:HG3	1.84	1.12
1:Q:11:GLN:NE2	2:R:247:GLN:O	1.83	1.12
1:A:346:TRP:HB2	2:P:401:ARG:CB	1.79	1.12
1:I:177:VAL:CG2	2:J:329:ASP:O	1.97	1.12
1:A:210:TYR:CZ	2:B:326:LYS:CA	2.33	1.12
2:J:283:TYR:CD2	2:L:62:VAL:HG22	1.84	1.12
1:C:101:ASN:N	2:D:254:LYS:HD2	1.65	1.11
1:C:133:GLN:NE2	2:N:97:SER:OG	1.83	1.11
2:P:283:TYR:C	2:R:56:ALA:HB1	1.70	1.11
1:E:97:GLU:OE2	2:F:2:ARG:NE	1.81	1.11
1:G:401:LYS:HG3	2:H:346:TRP:CB	1.81	1.11
1:O:181:VAL:CA	2:P:352:LYS:CE	2.08	1.11
1:A:404:PHE:H	2:B:261:PRO:HA	1.11	1.11
1:E:97:GLU:CD	2:F:2:ARG:NH2	2.04	1.11
1:O:96:LYS:O	2:P:2:ARG:HD2	1.47	1.11
1:Q:176:GLN:OE1	2:R:333:LEU:HD11	1.50	1.11
2:B:179:ASP:OD1	1:I:353:VAL:HB	1.51	1.10
1:E:353:VAL:HB	2:R:179:ASP:OD1	1.49	1.10
1:I:105:ARG:NH2	2:J:253:ARG:NH2	1.97	1.10
3:O:501:GTP:O3G	2:P:254:LYS:NZ	1.83	1.10
1:C:97:GLU:OE1	2:D:2:ARG:NH2	1.83	1.10
2:B:406:HIS:HE1	1:I:260:VAL:O	1.33	1.10
1:O:176:GLN:CB	2:P:333:LEU:CD2	2.13	1.10
1:Q:404:PHE:N	2:R:261:PRO:HA	1.65	1.10
1:A:210:TYR:CD1	2:B:326:LYS:HB2	1.86	1.10
2:B:403:ALA:CB	1:I:346:TRP:CE3	2.34	1.10
1:C:210:TYR:CZ	2:D:326:LYS:CA	2.35	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:GLU:CD	2:H:2:ARG:NH2	2.04	1.10
2:J:283:TYR:HD2	2:L:62:VAL:HG22	1.06	1.10
1:M:181:VAL:CA	2:N:352:LYS:CE	2.13	1.10
1:Q:181:VAL:CA	2:R:352:LYS:CE	2.11	1.10
1:E:210:TYR:CZ	2:F:326:LYS:CA	2.36	1.09
3:M:501:GTP:O3G	2:N:254:LYS:NZ	1.83	1.09
1:O:177:VAL:HG11	2:P:329:ASP:HA	1.23	1.09
1:A:105:ARG:NH2	2:B:253:ARG:NH2	1.99	1.09
2:B:283:TYR:HA	2:F:56:ALA:CB	1.82	1.09
1:C:404:PHE:H	2:D:261:PRO:HA	1.14	1.09
1:A:97:GLU:CD	2:B:2:ARG:NH2	2.06	1.09
1:E:133:GLN:NE2	2:R:97:SER:OG	1.85	1.09
2:F:181:VAL:CG2	1:K:350:GLY:O	2.00	1.09
1:A:181:VAL:CA	2:B:352:LYS:CE	2.24	1.09
1:C:210:TYR:CD1	2:D:326:LYS:HB2	1.87	1.09
1:Q:177:VAL:HG11	2:R:329:ASP:HA	1.29	1.09
2:B:406:HIS:CE1	1:I:260:VAL:O	2.05	1.08
3:K:501:GTP:O3G	2:L:254:LYS:NZ	1.85	1.08
1:O:283:HIS:HA	1:Q:56:THR:HG21	1.33	1.08
1:Q:404:PHE:H	2:R:261:PRO:HA	1.00	1.08
1:A:222:PRO:O	2:B:324:SER:HB2	1.54	1.08
1:E:97:GLU:OE1	2:F:2:ARG:NH2	1.85	1.08
1:K:224:TYR:CE1	2:L:325:MET:CG	2.35	1.08
1:O:404:PHE:H	2:P:261:PRO:CA	1.64	1.08
1:M:11:GLN:NE2	2:N:247:GLN:O	1.87	1.08
1:M:404:PHE:H	2:N:261:PRO:HA	0.97	1.08
2:D:179:ASP:OD1	1:G:353:VAL:HB	1.53	1.08
1:G:105:ARG:NH2	2:H:253:ARG:NH2	2.02	1.08
1:G:177:VAL:CG2	2:H:329:ASP:O	2.01	1.08
1:I:177:VAL:HG11	2:J:329:ASP:HA	1.31	1.08
1:K:177:VAL:CG2	2:L:329:ASP:O	2.01	1.08
1:M:96:LYS:O	2:N:2:ARG:HD2	1.50	1.08
1:Q:105:ARG:HH21	2:R:253:ARG:NH2	1.50	1.08
1:C:181:VAL:CA	2:D:352:LYS:CE	2.23	1.07
1:K:11:GLN:NE2	2:L:247:GLN:O	1.87	1.07
2:D:406:HIS:HE1	1:G:260:VAL:O	1.36	1.07
1:E:101:ASN:N	2:F:254:LYS:HD2	1.68	1.07
1:I:401:LYS:HG3	2:J:346:TRP:CB	1.83	1.07
1:O:404:PHE:H	2:P:261:PRO:HA	0.91	1.07
2:P:283:TYR:HA	2:R:56:ALA:HB3	1.37	1.07
1:Q:176:GLN:CB	2:R:333:LEU:CD2	2.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:210:TYR:CD2	2:R:326:LYS:HG3	1.89	1.07
1:A:283:HIS:HA	1:E:56:THR:HG21	1.33	1.07
1:G:404:PHE:H	2:H:261:PRO:HA	1.14	1.07
1:I:210:TYR:CD2	2:J:326:LYS:HG3	1.89	1.07
1:O:11:GLN:NE2	2:P:247:GLN:O	1.88	1.07
1:K:177:VAL:HG11	2:L:329:ASP:HA	1.34	1.07
1:O:406:HIS:CE1	2:P:260:VAL:O	2.08	1.07
1:Q:181:VAL:N	2:R:352:LYS:HE3	1.70	1.07
1:C:97:GLU:CD	2:D:2:ARG:NH2	2.08	1.06
2:F:179:ASP:OD1	1:K:353:VAL:HB	1.55	1.06
1:K:105:ARG:NH2	2:L:253:ARG:NH2	2.02	1.06
1:M:210:TYR:CD2	2:N:326:LYS:HG3	1.90	1.06
1:O:105:ARG:NH2	2:P:253:ARG:CZ	2.17	1.06
1:A:177:VAL:HG21	2:B:329:ASP:O	1.54	1.06
1:C:222:PRO:O	2:D:324:SER:HB2	1.56	1.06
2:H:283:TYR:CA	2:J:56:ALA:CB	2.33	1.06
1:I:224:TYR:CE1	2:J:325:MET:CG	2.36	1.06
1:K:401:LYS:HG3	2:L:346:TRP:CB	1.84	1.06
2:N:283:TYR:CA	2:P:56:ALA:CB	2.32	1.06
1:E:177:VAL:HG21	2:F:329:ASP:O	1.56	1.06
3:E:501:GTP:O3G	2:F:254:LYS:NZ	1.87	1.06
1:G:401:LYS:HD3	2:H:346:TRP:CE2	1.90	1.06
1:K:404:PHE:H	2:L:261:PRO:HA	1.14	1.06
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.04	1.06
1:C:346:TRP:CE3	2:N:403:ALA:CB	2.32	1.06
1:G:177:VAL:HG11	2:H:329:ASP:HA	1.34	1.06
1:M:177:VAL:HG11	2:N:329:ASP:HA	1.30	1.06
2:P:283:TYR:HD2	2:R:62:VAL:HG22	1.18	1.06
1:Q:96:LYS:O	2:R:2:ARG:HD2	1.54	1.06
1:E:401:LYS:HD3	2:F:346:TRP:CE2	1.89	1.05
3:I:501:GTP:O3G	2:J:254:LYS:NZ	1.88	1.05
1:O:394:LYS:HA	2:P:348:PRO:HG3	1.36	1.05
1:E:210:TYR:CD1	2:F:326:LYS:HB2	1.90	1.05
2:H:283:TYR:CD2	2:J:62:VAL:HG22	1.91	1.05
1:M:176:GLN:CB	2:N:333:LEU:CD2	2.19	1.05
1:O:404:PHE:CE2	2:P:258:ASN:O	2.10	1.05
2:F:403:ALA:CB	1:K:346:TRP:CE3	2.40	1.05
1:M:105:ARG:NH2	2:N:253:ARG:CZ	2.20	1.05
1:M:404:PHE:H	2:N:261:PRO:CA	1.68	1.05
2:D:406:HIS:CE1	1:G:260:VAL:O	2.09	1.05
1:A:56:THR:HG21	1:C:283:HIS:HA	1.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TRP:HB2	2:P:401:ARG:HB2	1.33	1.05
1:C:177:VAL:HG21	2:D:329:ASP:C	1.75	1.05
1:E:222:PRO:O	2:F:324:SER:HB2	1.57	1.05
1:I:181:VAL:CB	2:J:352:LYS:HE3	1.86	1.05
1:A:177:VAL:HG21	2:B:329:ASP:C	1.75	1.04
1:C:346:TRP:HB2	2:N:401:ARG:CB	1.86	1.04
1:E:11:GLN:NE2	2:F:247:GLN:O	1.89	1.04
2:F:406:HIS:HE1	1:K:260:VAL:O	1.39	1.04
3:G:501:GTP:O3G	2:H:254:LYS:NZ	1.90	1.04
1:I:11:GLN:NE2	2:J:247:GLN:O	1.91	1.04
2:J:283:TYR:C	2:L:56:ALA:HB1	1.78	1.04
1:A:105:ARG:HH21	2:B:253:ARG:NH2	1.54	1.04
1:G:181:VAL:CB	2:H:352:LYS:HE3	1.85	1.04
1:K:401:LYS:HD3	2:L:346:TRP:CE2	1.90	1.04
1:O:401:LYS:HG3	2:P:346:TRP:CB	1.87	1.04
1:A:96:LYS:O	2:B:2:ARG:HD2	1.57	1.04
2:B:97:SER:OG	1:I:133:GLN:NE2	1.90	1.04
1:E:177:VAL:HG21	2:F:329:ASP:C	1.78	1.04
1:E:401:LYS:HG3	2:F:346:TRP:CB	1.87	1.04
1:G:224:TYR:CE1	2:H:325:MET:CG	2.39	1.04
1:I:283:HIS:HA	1:K:56:THR:HG21	1.39	1.04
1:K:210:TYR:CD2	2:L:326:LYS:HG3	1.93	1.04
1:A:2:ARG:NH1	2:P:72:PRO:HB2	1.73	1.04
2:B:56:ALA:CB	2:D:283:TYR:HA	1.88	1.04
1:G:210:TYR:CD2	2:H:326:LYS:HG3	1.93	1.04
1:I:176:GLN:OE1	2:J:333:LEU:HD11	1.56	1.04
1:K:224:TYR:CD1	2:L:325:MET:HG3	1.92	1.03
1:K:401:LYS:HG3	2:L:346:TRP:CG	1.92	1.03
1:O:100:ALA:CA	2:P:254:LYS:HB2	1.87	1.03
1:C:177:VAL:HG21	2:D:329:ASP:O	1.56	1.03
1:E:401:LYS:HG3	2:F:346:TRP:CG	1.92	1.03
1:I:406:HIS:CE1	2:J:260:VAL:O	2.11	1.03
1:K:181:VAL:N	2:L:352:LYS:HE3	1.71	1.03
1:E:404:PHE:H	2:F:261:PRO:HA	1.19	1.03
2:D:97:SER:OG	1:G:133:GLN:NE2	1.89	1.03
2:N:283:TYR:C	2:P:56:ALA:HB1	1.76	1.03
1:G:283:HIS:HA	1:I:56:THR:HG21	1.41	1.03
1:K:181:VAL:CB	2:L:352:LYS:HE3	1.87	1.03
1:O:101:ASN:HB2	2:P:254:LYS:CD	1.88	1.03
1:O:394:LYS:CA	2:P:348:PRO:HG3	1.87	1.03
1:O:394:LYS:NZ	2:P:349:ASN:HD21	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:HIS:CE1	2:H:260:VAL:O	2.12	1.02
1:K:224:TYR:CE1	2:L:325:MET:HG3	1.93	1.02
1:M:283:HIS:HA	1:O:56:THR:HG21	1.42	1.02
2:N:283:TYR:HD2	2:P:62:VAL:HG22	1.20	1.02
1:Q:105:ARG:NH2	2:R:253:ARG:CZ	2.22	1.02
1:E:260:VAL:HB	2:R:407:TRP:CZ2	1.94	1.02
2:F:97:SER:OG	1:K:133:GLN:NE2	1.92	1.02
1:G:401:LYS:HG3	2:H:346:TRP:CG	1.94	1.02
1:E:181:VAL:N	2:F:352:LYS:HE3	1.72	1.02
2:J:283:TYR:HA	2:L:56:ALA:HB3	1.40	1.02
1:K:176:GLN:CB	2:L:333:LEU:CD2	2.22	1.02
1:K:406:HIS:CE1	2:L:260:VAL:O	2.13	1.02
1:Q:404:PHE:H	2:R:261:PRO:CA	1.69	1.02
1:I:401:LYS:HD3	2:J:346:TRP:CE2	1.93	1.02
1:O:210:TYR:CE1	2:P:326:LYS:CB	2.43	1.02
1:C:401:LYS:HG3	2:D:346:TRP:CB	1.90	1.01
1:G:11:GLN:NE2	2:H:247:GLN:O	1.93	1.01
1:G:176:GLN:OE1	2:H:333:LEU:HD11	1.59	1.01
1:I:224:TYR:CE1	2:J:325:MET:HG3	1.94	1.01
1:O:210:TYR:OH	2:P:326:LYS:N	1.92	1.01
1:C:346:TRP:HB2	2:N:401:ARG:HB2	1.39	1.01
2:P:283:TYR:CD2	2:R:62:VAL:HG22	1.95	1.01
1:A:406:HIS:CE1	2:B:260:VAL:HG12	1.94	1.01
1:E:105:ARG:NH2	2:F:253:ARG:NH2	2.08	1.01
1:A:350:GLY:HA3	2:P:181:VAL:HA	1.41	1.01
1:M:181:VAL:N	2:N:352:LYS:HE3	1.75	1.01
1:Q:406:HIS:CE1	2:R:260:VAL:O	2.14	1.01
3:A:501:GTP:O3G	2:B:254:LYS:NZ	1.92	1.01
1:C:105:ARG:HH21	2:D:253:ARG:HH21	1.04	1.01
1:C:105:ARG:HH21	2:D:253:ARG:NH2	1.59	1.01
2:D:403:ALA:CB	1:G:346:TRP:CE3	2.40	1.01
1:M:406:HIS:CE1	2:N:260:VAL:O	2.13	1.01
1:A:11:GLN:NE2	2:B:247:GLN:O	1.93	1.00
1:A:260:VAL:HB	2:P:407:TRP:CZ2	1.95	1.00
1:A:346:TRP:CB	2:P:401:ARG:CB	2.39	1.00
2:F:406:HIS:CE1	1:K:260:VAL:O	2.13	1.00
1:G:224:TYR:CE1	2:H:325:MET:HG3	1.96	1.00
1:I:96:LYS:O	2:J:2:ARG:HD2	1.59	1.00
1:M:394:LYS:HA	2:N:348:PRO:HG3	1.39	1.00
1:M:394:LYS:CA	2:N:348:PRO:HG3	1.91	1.00
1:O:181:VAL:N	2:P:352:LYS:HE3	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:ARG:HH21	2:J:253:ARG:NH2	1.57	1.00
1:M:101:ASN:HB2	2:N:254:LYS:CD	1.91	1.00
1:Q:210:TYR:CE1	2:R:326:LYS:CB	2.44	1.00
1:C:406:HIS:CE1	2:D:260:VAL:HG12	1.96	1.00
3:C:501:GTP:O3G	2:D:254:LYS:NZ	1.92	1.00
1:E:346:TRP:HB2	2:R:401:ARG:CB	1.92	1.00
1:A:404:PHE:N	2:B:261:PRO:HA	1.77	1.00
1:C:2:ARG:NH1	2:N:72:PRO:HB2	1.77	1.00
1:G:401:LYS:CG	2:H:346:TRP:CG	2.45	1.00
1:O:210:TYR:CE2	2:P:326:LYS:CA	2.37	1.00
1:O:181:VAL:CB	2:P:352:LYS:HE3	1.92	0.99
1:I:401:LYS:HG3	2:J:346:TRP:CG	1.96	0.99
1:M:401:LYS:HG3	2:N:346:TRP:CB	1.91	0.99
1:C:11:GLN:NE2	2:D:247:GLN:O	1.94	0.99
1:M:100:ALA:CA	2:N:254:LYS:HB2	1.91	0.99
1:O:210:TYR:HB3	2:P:326:LYS:HD2	1.44	0.99
1:Q:401:LYS:HG3	2:R:346:TRP:CB	1.91	0.99
1:E:346:TRP:HB2	2:R:401:ARG:HB2	1.42	0.99
1:E:406:HIS:CE1	2:F:260:VAL:HG12	1.98	0.99
1:O:394:LYS:HG2	2:P:348:PRO:HB2	1.42	0.99
1:I:224:TYR:CD1	2:J:325:MET:HG3	1.97	0.99
1:C:401:LYS:HD3	2:D:346:TRP:CE2	1.97	0.99
1:Q:401:LYS:HG3	2:R:346:TRP:CG	1.98	0.99
2:D:403:ALA:HB1	1:G:346:TRP:HZ3	1.19	0.99
1:G:181:VAL:N	2:H:352:LYS:HE3	1.76	0.99
1:O:401:LYS:CG	2:P:346:TRP:CG	2.45	0.99
1:A:177:VAL:CG2	2:B:329:ASP:O	2.11	0.99
1:I:406:HIS:CE1	2:J:260:VAL:HG12	1.95	0.99
1:K:401:LYS:CG	2:L:346:TRP:CG	2.45	0.99
2:N:283:TYR:HA	2:P:56:ALA:HB3	1.44	0.99
1:I:176:GLN:CB	2:J:333:LEU:CD2	2.21	0.99
2:J:283:TYR:CA	2:L:56:ALA:HB1	1.93	0.99
1:Q:394:LYS:CA	2:R:348:PRO:HG3	1.92	0.99
1:E:181:VAL:CB	2:F:352:LYS:HE3	1.91	0.98
1:E:224:TYR:CE1	2:F:325:MET:CG	2.46	0.98
1:I:181:VAL:N	2:J:352:LYS:HE3	1.76	0.98
1:I:407:TRP:CE2	2:J:257:VAL:HA	1.98	0.98
1:A:258:ASN:C	2:P:404:PHE:HE2	1.65	0.98
2:B:283:TYR:HD2	2:F:62:VAL:HG22	1.28	0.98
1:E:224:TYR:CD1	2:F:325:MET:HG3	1.99	0.98
1:K:176:GLN:OE1	2:L:333:LEU:HD11	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:OE1	2:B:333:LEU:HD11	1.62	0.98
1:I:406:HIS:HE1	2:J:260:VAL:O	1.45	0.98
1:M:210:TYR:CE1	2:N:326:LYS:CB	2.46	0.98
1:K:406:HIS:CE1	2:L:260:VAL:HG12	1.97	0.98
1:Q:394:LYS:HA	2:R:348:PRO:HG3	1.42	0.98
2:N:283:TYR:CD2	2:P:62:VAL:HG22	1.99	0.98
1:C:96:LYS:O	2:D:2:ARG:HD2	1.63	0.98
1:Q:401:LYS:CG	2:R:346:TRP:CG	2.47	0.98
1:A:105:ARG:HH21	2:B:253:ARG:HH21	0.99	0.98
1:A:283:HIS:CA	1:E:56:THR:HG21	1.94	0.98
1:A:348:PRO:HD3	2:P:398:MET:CG	1.94	0.98
1:I:401:LYS:CG	2:J:346:TRP:CG	2.46	0.98
1:K:97:GLU:OE2	2:L:2:ARG:NH2	1.95	0.98
1:M:394:LYS:HG2	2:N:348:PRO:HB2	1.46	0.98
1:O:101:ASN:CG	2:P:254:LYS:HE3	1.82	0.98
1:O:210:TYR:HB3	2:P:326:LYS:CD	1.92	0.98
1:Q:224:TYR:CG	2:R:325:MET:HG3	1.97	0.98
1:M:210:TYR:CE2	2:N:326:LYS:CA	2.43	0.98
2:P:283:TYR:C	2:R:56:ALA:CB	2.28	0.97
1:A:348:PRO:CD	2:P:398:MET:CG	2.42	0.97
1:Q:100:ALA:CA	2:R:254:LYS:HB2	1.92	0.97
1:A:352:LYS:HA	2:P:179:ASP:O	1.63	0.97
1:E:2:ARG:NH1	2:R:72:PRO:HB2	1.80	0.97
1:E:177:VAL:HG11	2:F:329:ASP:HA	1.45	0.97
1:G:406:HIS:HE1	2:H:260:VAL:O	1.46	0.97
1:G:407:TRP:CE2	2:H:257:VAL:HA	1.99	0.97
1:I:404:PHE:N	2:J:261:PRO:HA	1.79	0.97
1:E:105:ARG:HH21	2:F:253:ARG:HH21	1.08	0.97
1:M:404:PHE:CE2	2:N:258:ASN:O	2.17	0.97
2:P:284:ARG:O	2:R:57:ALA:N	1.95	0.97
1:C:404:PHE:N	2:D:261:PRO:HA	1.80	0.97
1:G:224:TYR:CD1	2:H:325:MET:HG3	1.99	0.97
1:I:210:TYR:CE1	2:J:326:LYS:CB	2.48	0.97
1:A:401:LYS:HG3	2:B:346:TRP:CB	1.93	0.97
1:C:177:VAL:CG2	2:D:329:ASP:O	2.12	0.97
1:A:224:TYR:CE1	2:B:325:MET:CG	2.47	0.97
1:C:181:VAL:CB	2:D:352:LYS:HE3	1.94	0.97
1:G:105:ARG:HH21	2:H:253:ARG:NH2	1.61	0.97
1:A:177:VAL:HG11	2:B:329:ASP:HA	1.44	0.96
1:E:406:HIS:CE1	2:F:260:VAL:O	2.18	0.96
2:H:283:TYR:C	2:J:56:ALA:HB1	1.84	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:401:LYS:HD3	2:R:346:TRP:CE2	1.99	0.96
1:A:346:TRP:HE3	2:P:403:ALA:HB2	1.26	0.96
1:C:260:VAL:HB	2:N:407:TRP:CZ2	1.99	0.96
1:O:97:GLU:OE2	2:P:2:ARG:CZ	2.12	0.96
1:E:401:LYS:CG	2:F:346:TRP:CG	2.47	0.96
2:J:283:TYR:C	2:L:56:ALA:CB	2.34	0.96
1:M:210:TYR:OH	2:N:326:LYS:N	1.98	0.96
2:B:401:ARG:CB	1:I:346:TRP:HB2	1.95	0.96
1:C:176:GLN:OE1	2:D:333:LEU:HD11	1.64	0.96
1:I:210:TYR:HB3	2:J:326:LYS:HD2	1.47	0.96
2:B:401:ARG:HB2	1:I:346:TRP:HB2	1.46	0.96
1:G:406:HIS:CE1	2:H:260:VAL:HG12	1.99	0.96
1:M:394:LYS:NZ	2:N:349:ASN:HD21	1.63	0.96
1:O:407:TRP:CE2	2:P:257:VAL:HA	2.01	0.96
1:K:96:LYS:O	2:L:2:ARG:HD2	1.64	0.96
1:K:97:GLU:OE2	2:L:2:ARG:CZ	2.12	0.96
1:O:397:LEU:HB3	2:P:346:TRP:O	1.66	0.96
1:A:176:GLN:HB3	2:B:333:LEU:HD22	0.96	0.96
1:K:105:ARG:HH21	2:L:253:ARG:NH2	1.62	0.96
1:O:283:HIS:CA	1:Q:56:THR:HG21	1.95	0.96
1:A:105:ARG:NH2	2:B:253:ARG:CZ	2.29	0.96
1:C:350:GLY:HA3	2:N:181:VAL:HA	1.47	0.96
1:E:96:LYS:O	2:F:2:ARG:HD2	1.66	0.96
1:G:96:LYS:O	2:H:2:ARG:HD2	1.63	0.96
1:I:210:TYR:CE2	2:J:326:LYS:CA	2.44	0.96
1:Q:181:VAL:CB	2:R:352:LYS:HE3	1.95	0.96
1:A:406:HIS:CE1	2:B:260:VAL:O	2.19	0.95
1:E:105:ARG:HH21	2:F:253:ARG:NH2	1.63	0.95
1:E:177:VAL:CG2	2:F:329:ASP:O	2.13	0.95
2:H:283:TYR:HA	2:J:56:ALA:HB3	1.48	0.95
1:O:101:ASN:N	2:P:254:LYS:CD	2.29	0.95
1:C:406:HIS:CE1	2:D:260:VAL:O	2.19	0.95
1:M:401:LYS:CG	2:N:346:TRP:CG	2.49	0.95
1:G:176:GLN:CB	2:H:333:LEU:CD2	2.24	0.95
1:Q:394:LYS:HG2	2:R:348:PRO:HB2	1.47	0.95
1:Q:394:LYS:NZ	2:R:349:ASN:HD21	1.64	0.95
2:B:62:VAL:HG22	2:D:283:TYR:HD2	1.31	0.95
1:G:210:TYR:CE2	2:H:326:LYS:CA	2.46	0.95
1:G:210:TYR:HB3	2:H:326:LYS:HD2	1.48	0.95
1:I:224:TYR:CZ	2:J:325:MET:HG3	1.99	0.95
1:I:404:PHE:CE2	2:J:258:ASN:O	2.20	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:HIS:HE1	2:N:260:VAL:O	1.48	0.95
1:A:181:VAL:CB	2:B:352:LYS:HE3	1.95	0.95
1:C:401:LYS:HG3	2:D:346:TRP:CG	2.00	0.95
1:M:181:VAL:CB	2:N:352:LYS:HE3	1.96	0.95
1:O:394:LYS:NZ	2:P:349:ASN:ND2	2.15	0.95
1:O:401:LYS:HG3	2:P:346:TRP:CG	2.01	0.95
1:C:177:VAL:HG11	2:D:329:ASP:HA	1.45	0.95
1:I:210:TYR:OH	2:J:326:LYS:N	1.99	0.95
2:N:284:ARG:O	2:P:57:ALA:N	1.99	0.95
1:O:210:TYR:CZ	2:P:326:LYS:N	2.33	0.95
1:Q:97:GLU:OE2	2:R:2:ARG:CZ	2.14	0.95
1:A:348:PRO:CD	2:P:398:MET:HG2	1.96	0.95
1:I:97:GLU:OE2	2:J:2:ARG:NH2	2.00	0.95
1:K:210:TYR:CE1	2:L:326:LYS:CB	2.49	0.95
1:K:407:TRP:CE2	2:L:257:VAL:HA	2.01	0.95
2:B:407:TRP:CZ2	1:I:260:VAL:HB	2.02	0.95
1:E:97:GLU:OE2	2:F:2:ARG:NH2	1.97	0.95
1:Q:394:LYS:HZ1	2:R:349:ASN:HD21	0.99	0.95
1:E:224:TYR:CE1	2:F:325:MET:HG3	2.01	0.95
1:E:401:LYS:HE2	2:F:346:TRP:CD1	2.02	0.95
1:O:179:THR:HG21	2:P:353:THR:OG1	1.67	0.95
1:C:181:VAL:N	2:D:352:LYS:HE3	1.80	0.95
1:C:224:TYR:CE1	2:D:325:MET:CG	2.50	0.95
1:I:97:GLU:OE2	2:J:2:ARG:CZ	2.13	0.95
1:Q:210:TYR:OH	2:R:326:LYS:N	1.99	0.95
1:A:101:ASN:HB2	2:B:254:LYS:CD	1.95	0.94
1:A:181:VAL:N	2:B:352:LYS:HE3	1.81	0.94
1:K:406:HIS:HE1	2:L:260:VAL:O	1.48	0.94
1:M:224:TYR:CG	2:N:325:MET:HG3	2.01	0.94
1:M:401:LYS:HG3	2:N:346:TRP:CG	2.02	0.94
1:O:401:LYS:HD3	2:P:346:TRP:CE2	2.02	0.94
1:C:176:GLN:HB3	2:D:333:LEU:HD22	0.95	0.94
1:M:210:TYR:HB3	2:N:326:LYS:HD2	1.49	0.94
1:Q:404:PHE:CE2	2:R:258:ASN:O	2.20	0.94
1:C:352:LYS:HA	2:N:179:ASP:O	1.66	0.94
1:K:105:ARG:HH21	2:L:253:ARG:HH21	1.01	0.94
1:O:404:PHE:HZ	2:P:314:THR:CG2	1.79	0.94
1:K:224:TYR:CG	2:L:325:MET:HG3	2.02	0.94
1:Q:97:GLU:OE2	2:R:2:ARG:NH2	1.99	0.94
1:A:394:LYS:HA	2:B:348:PRO:HG3	1.50	0.94
1:G:401:LYS:HE2	2:H:346:TRP:CD1	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:404:PHE:N	2:H:261:PRO:HA	1.82	0.94
1:M:101:ASN:CG	2:N:254:LYS:HE3	1.87	0.94
1:C:258:ASN:C	2:N:404:PHE:HE2	1.70	0.94
1:G:224:TYR:CZ	2:H:325:MET:HG3	2.01	0.94
1:G:401:LYS:HG3	2:H:346:TRP:HB3	1.46	0.94
1:K:404:PHE:N	2:L:261:PRO:HA	1.81	0.94
1:M:397:LEU:HB3	2:N:346:TRP:O	1.68	0.94
2:N:283:TYR:C	2:P:56:ALA:CB	2.35	0.94
1:O:176:GLN:CG	2:P:333:LEU:HD21	1.97	0.94
1:I:101:ASN:HB2	2:J:254:LYS:CD	1.96	0.94
1:O:407:TRP:CD2	2:P:257:VAL:HA	2.03	0.94
1:A:348:PRO:HD3	2:P:398:MET:HG2	1.49	0.94
1:E:346:TRP:HE3	2:R:403:ALA:HB2	1.31	0.94
2:F:403:ALA:HB1	1:K:346:TRP:HZ3	1.22	0.94
1:O:101:ASN:CB	2:P:254:LYS:CE	2.20	0.94
2:B:403:ALA:HB1	1:I:346:TRP:HZ3	1.13	0.93
1:C:346:TRP:CB	2:N:401:ARG:CB	2.46	0.93
1:E:176:GLN:HB3	2:F:333:LEU:HD22	0.96	0.93
1:G:401:LYS:HD3	2:H:346:TRP:CD2	2.03	0.93
1:M:401:LYS:HD3	2:N:346:TRP:CE2	2.03	0.93
1:I:210:TYR:HB3	2:J:326:LYS:CD	1.97	0.93
1:Q:101:ASN:HB2	2:R:254:LYS:CD	1.97	0.93
1:O:224:TYR:CD2	2:P:325:MET:HG3	2.03	0.93
1:A:224:TYR:CD1	2:B:325:MET:HG3	2.03	0.93
1:A:346:TRP:CB	2:P:401:ARG:CG	2.25	0.93
2:B:283:TYR:C	2:F:56:ALA:HB1	1.87	0.93
1:O:224:TYR:CG	2:P:325:MET:HG3	2.01	0.93
1:O:406:HIS:HE1	2:P:260:VAL:O	1.42	0.93
1:A:224:TYR:CE1	2:B:325:MET:HG3	2.03	0.93
2:B:283:TYR:CA	2:F:56:ALA:CB	2.46	0.93
1:C:105:ARG:NH2	2:D:253:ARG:CZ	2.32	0.93
1:E:350:GLY:HA3	2:R:181:VAL:HA	1.50	0.93
1:M:210:TYR:HB3	2:N:326:LYS:CD	1.97	0.93
1:I:394:LYS:HA	2:J:348:PRO:HG3	1.51	0.93
1:I:401:LYS:HG3	2:J:346:TRP:HB3	1.49	0.93
1:M:97:GLU:OE2	2:N:2:ARG:CZ	2.16	0.93
1:M:179:THR:HG21	2:N:353:THR:OG1	1.69	0.93
1:E:224:TYR:HE1	2:F:325:MET:SD	1.87	0.93
1:O:177:VAL:HG11	2:P:329:ASP:CA	1.99	0.93
2:B:72:PRO:HB2	1:I:2:ARG:NH1	1.83	0.93
1:G:404:PHE:CE2	2:H:258:ASN:O	2.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:TYR:CZ	2:L:325:MET:HG3	2.03	0.93
1:M:394:LYS:HZ1	2:N:349:ASN:ND2	1.67	0.93
1:E:404:PHE:N	2:F:261:PRO:HA	1.83	0.93
2:P:283:TYR:CA	2:R:56:ALA:HB1	1.94	0.93
1:A:401:LYS:HD3	2:B:346:TRP:CE2	2.03	0.93
1:E:348:PRO:HD3	2:R:398:MET:CG	1.98	0.93
1:G:210:TYR:CE1	2:H:326:LYS:CB	2.52	0.93
1:I:105:ARG:NH2	2:J:253:ARG:CZ	2.31	0.93
1:K:401:LYS:HE2	2:L:346:TRP:CD1	2.04	0.93
2:D:72:PRO:HB2	1:G:2:ARG:NH1	1.83	0.92
1:M:179:THR:HG22	2:N:353:THR:HG1	1.31	0.92
1:G:105:ARG:HH21	2:H:253:ARG:HH21	1.01	0.92
1:G:97:GLU:OE2	2:H:2:ARG:NH2	2.00	0.92
1:I:105:ARG:HH21	2:J:253:ARG:HH21	0.96	0.92
1:O:210:TYR:HB3	2:P:326:LYS:CE	1.98	0.92
1:G:97:GLU:OE2	2:H:2:ARG:CZ	2.16	0.92
1:I:283:HIS:CA	1:K:56:THR:HG21	1.99	0.92
1:Q:404:PHE:HZ	2:R:314:THR:CG2	1.82	0.92
1:A:249:ASN:H	2:P:11:GLN:HE22	1.17	0.92
1:E:105:ARG:NH2	2:F:253:ARG:CZ	2.33	0.92
1:Q:179:THR:HG21	2:R:353:THR:OG1	1.68	0.92
1:C:348:PRO:HD3	2:N:398:MET:CG	1.99	0.92
1:I:224:TYR:CG	2:J:325:MET:HG3	2.05	0.92
1:K:401:LYS:HG3	2:L:346:TRP:HB3	1.51	0.92
1:Q:210:TYR:HB3	2:R:326:LYS:CD	1.99	0.92
1:C:224:TYR:CE1	2:D:325:MET:HG3	2.05	0.92
2:D:401:ARG:HB2	1:G:346:TRP:HB2	1.52	0.92
1:M:404:PHE:HZ	2:N:314:THR:CG2	1.82	0.92
2:F:72:PRO:HB2	1:K:2:ARG:NH1	1.85	0.92
1:G:210:TYR:HB3	2:H:326:LYS:CD	2.00	0.92
1:C:348:PRO:CD	2:N:398:MET:CG	2.48	0.91
1:I:100:ALA:CA	2:J:254:LYS:HB2	2.00	0.91
1:K:210:TYR:OH	2:L:326:LYS:N	2.03	0.91
1:O:96:LYS:O	2:P:2:ARG:CD	2.18	0.91
1:Q:210:TYR:HB3	2:R:326:LYS:HD2	1.52	0.91
1:G:101:ASN:HB2	2:H:254:LYS:CD	1.98	0.91
1:G:210:TYR:OH	2:H:326:LYS:N	2.02	0.91
1:G:224:TYR:HE1	2:H:325:MET:SD	1.81	0.91
1:M:210:TYR:CZ	2:N:326:LYS:N	2.37	0.91
1:O:179:THR:HA	2:P:353:THR:H	1.35	0.91
1:C:224:TYR:CD1	2:D:325:MET:HG3	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:210:TYR:CZ	2:P:326:LYS:CB	2.53	0.91
1:A:401:LYS:HG3	2:B:346:TRP:CG	2.05	0.91
1:C:101:ASN:HB2	2:D:254:LYS:CD	1.99	0.91
1:Q:210:TYR:CE2	2:R:326:LYS:CA	2.45	0.91
1:C:346:TRP:CB	2:N:401:ARG:CG	2.30	0.91
1:A:404:PHE:H	2:B:261:PRO:CA	1.83	0.91
1:I:224:TYR:HE1	2:J:325:MET:SD	1.77	0.91
1:Q:105:ARG:HH21	2:R:253:ARG:HH21	0.93	0.91
1:G:401:LYS:CE	2:H:346:TRP:CD1	2.53	0.91
2:H:283:TYR:CA	2:J:56:ALA:HB1	2.01	0.91
1:I:101:ASN:CG	2:J:254:LYS:HE3	1.91	0.91
1:O:100:ALA:HA	2:P:254:LYS:CB	2.01	0.91
1:C:101:ASN:HB2	2:D:254:LYS:HE3	0.91	0.91
1:C:401:LYS:CG	2:D:346:TRP:CG	2.53	0.91
2:P:284:ARG:N	2:R:56:ALA:HB1	1.86	0.91
1:Q:406:HIS:HE1	2:R:260:VAL:O	1.49	0.91
1:C:394:LYS:HA	2:D:348:PRO:HG3	1.53	0.91
2:D:401:ARG:CB	1:G:346:TRP:HB2	2.01	0.91
2:F:407:TRP:CZ2	1:K:260:VAL:HB	2.06	0.91
1:I:224:TYR:CZ	2:J:325:MET:SD	2.63	0.91
1:K:105:ARG:NH2	2:L:253:ARG:CZ	2.33	0.91
1:M:224:TYR:CD2	2:N:325:MET:HG3	2.06	0.91
1:M:407:TRP:CE2	2:N:257:VAL:HA	2.06	0.91
1:O:97:GLU:CD	2:P:2:ARG:HE	1.73	0.91
1:C:346:TRP:HE3	2:N:403:ALA:HB2	1.33	0.90
1:M:96:LYS:O	2:N:2:ARG:CD	2.19	0.90
1:O:406:HIS:NE2	2:P:260:VAL:CG1	2.34	0.90
1:Q:224:TYR:CD2	2:R:325:MET:HG3	2.05	0.90
1:A:210:TYR:CD2	2:B:326:LYS:HG3	2.06	0.90
2:B:56:ALA:HB1	2:D:283:TYR:C	1.90	0.90
1:E:176:GLN:OE1	2:F:333:LEU:HD11	1.70	0.90
2:F:228:ASN:HD21	5:F:901:GDP:HN1	1.17	0.90
1:K:224:TYR:CD1	2:L:325:MET:CG	2.52	0.90
2:L:228:ASN:HD21	5:L:901:GDP:HN1	1.17	0.90
1:O:224:TYR:CE2	2:P:325:MET:HG3	2.01	0.90
1:A:56:THR:HG21	1:C:283:HIS:CA	2.00	0.90
1:A:101:ASN:HB2	2:B:254:LYS:HE3	0.91	0.90
1:A:101:ASN:CG	2:B:254:LYS:HE3	1.91	0.90
2:B:284:ARG:O	2:F:57:ALA:N	2.04	0.90
2:N:228:ASN:HD21	5:N:901:GDP:HN1	1.17	0.90
1:O:394:LYS:HZ1	2:P:349:ASN:ND2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.06	0.90
1:M:101:ASN:CB	2:N:254:LYS:CE	2.27	0.90
1:Q:406:HIS:NE2	2:R:260:VAL:HG12	1.85	0.90
2:D:228:ASN:HD21	5:D:901:GDP:HN1	1.17	0.90
1:E:346:TRP:CB	2:R:401:ARG:CB	2.50	0.90
2:H:228:ASN:HD21	5:H:901:GDP:HN1	1.17	0.90
2:J:283:TYR:HB3	2:L:62:VAL:HG21	1.51	0.90
1:M:394:LYS:NZ	2:N:349:ASN:ND2	2.19	0.90
1:A:406:HIS:HE1	2:B:260:VAL:O	1.52	0.90
2:B:179:ASP:O	1:I:352:LYS:HA	1.70	0.90
2:D:407:TRP:CZ2	1:G:260:VAL:HB	2.07	0.90
1:G:105:ARG:NH2	2:H:253:ARG:CZ	2.35	0.90
1:I:224:TYR:CZ	2:J:325:MET:CG	2.55	0.90
1:I:401:LYS:HD3	2:J:346:TRP:CD2	2.07	0.90
1:M:105:ARG:HH21	2:N:253:ARG:HH21	0.90	0.90
1:O:97:GLU:OE2	2:P:2:ARG:NH2	2.03	0.90
2:N:283:TYR:CA	2:P:56:ALA:HB1	2.00	0.90
1:Q:176:GLN:HB2	2:R:333:LEU:HD22	1.51	0.90
2:R:228:ASN:HD21	5:R:901:GDP:HN1	1.17	0.90
1:I:394:LYS:NZ	2:J:349:ASN:HD21	1.70	0.90
1:A:404:PHE:CE2	2:B:258:ASN:O	2.25	0.90
2:B:181:VAL:HA	1:I:350:GLY:HA3	1.54	0.90
1:I:401:LYS:HE2	2:J:346:TRP:CD1	2.07	0.90
1:I:404:PHE:H	2:J:261:PRO:CA	1.84	0.90
1:O:404:PHE:HZ	2:P:314:THR:HG22	1.36	0.90
1:O:406:HIS:NE2	2:P:260:VAL:HG12	1.85	0.90
1:Q:210:TYR:CZ	2:R:326:LYS:N	2.39	0.90
1:Q:210:TYR:HB3	2:R:326:LYS:CE	2.01	0.90
2:B:283:TYR:CD2	2:F:62:VAL:HG22	2.07	0.89
1:K:404:PHE:CE2	2:L:258:ASN:O	2.25	0.89
1:E:352:LYS:HA	2:R:179:ASP:O	1.70	0.89
1:Q:176:GLN:CG	2:R:333:LEU:HD21	2.02	0.89
1:E:101:ASN:HB2	2:F:254:LYS:HE3	0.91	0.89
1:O:210:TYR:CB	2:P:326:LYS:HD2	2.02	0.89
1:K:210:TYR:CE2	2:L:326:LYS:CA	2.50	0.89
1:C:210:TYR:CD2	2:D:326:LYS:HG3	2.08	0.89
1:E:210:TYR:CD2	2:F:326:LYS:HG3	2.08	0.89
1:Q:397:LEU:HB3	2:R:346:TRP:O	1.73	0.89
1:E:401:LYS:HG3	2:F:346:TRP:HB3	1.54	0.89
1:I:210:TYR:CZ	2:J:326:LYS:N	2.39	0.89
1:K:210:TYR:HB3	2:L:326:LYS:HD2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:ASN:N	2:N:254:LYS:CD	2.34	0.89
1:O:176:GLN:HB2	2:P:333:LEU:HD22	1.50	0.89
1:Q:101:ASN:CG	2:R:254:LYS:HE3	1.92	0.89
1:C:406:HIS:HE1	2:D:260:VAL:O	1.54	0.89
1:E:348:PRO:CD	2:R:398:MET:CG	2.50	0.89
1:K:100:ALA:CA	2:L:254:LYS:HB2	2.02	0.89
1:A:97:GLU:OE2	2:B:2:ARG:NH2	2.05	0.89
2:D:179:ASP:O	1:G:352:LYS:HA	1.72	0.89
2:F:401:ARG:HB2	1:K:346:TRP:HB2	1.55	0.89
1:I:407:TRP:CD2	2:J:257:VAL:HA	2.08	0.89
1:M:97:GLU:OE2	2:N:2:ARG:NH2	2.03	0.89
1:Q:394:LYS:NZ	2:R:349:ASN:ND2	2.21	0.89
1:C:404:PHE:H	2:D:261:PRO:CA	1.85	0.89
1:E:258:ASN:C	2:R:404:PHE:HE2	1.76	0.89
1:G:224:TYR:CG	2:H:325:MET:HG3	2.08	0.89
1:G:394:LYS:HA	2:H:348:PRO:HG3	1.55	0.89
1:K:401:LYS:CE	2:L:346:TRP:CD1	2.55	0.89
2:P:228:ASN:HD21	5:P:901:GDP:HN1	1.17	0.89
1:C:97:GLU:OE2	2:D:2:ARG:NH2	2.05	0.88
1:C:346:TRP:HZ3	2:N:403:ALA:HB1	1.05	0.88
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.07	0.88
1:I:177:VAL:HG11	2:J:329:ASP:CA	2.03	0.88
1:I:401:LYS:CE	2:J:346:TRP:CD1	2.56	0.88
1:M:176:GLN:CG	2:N:333:LEU:HD21	2.03	0.88
1:M:176:GLN:HB2	2:N:333:LEU:HD22	1.54	0.88
1:Q:407:TRP:CE2	2:R:257:VAL:HA	2.07	0.88
1:A:394:LYS:HZ1	2:B:349:ASN:HD21	1.22	0.88
1:K:401:LYS:HD3	2:L:346:TRP:CD2	2.08	0.88
1:I:224:TYR:CE2	2:J:325:MET:HG3	2.08	0.88
2:J:284:ARG:O	2:L:57:ALA:N	2.05	0.88
1:O:176:GLN:CG	2:P:333:LEU:CD2	2.51	0.88
2:B:228:ASN:HD21	5:B:901:GDP:HN1	1.17	0.88
1:E:401:LYS:HD3	2:F:346:TRP:CD2	2.08	0.88
1:G:101:ASN:CG	2:H:254:LYS:HE3	1.94	0.88
1:M:406:HIS:NE2	2:N:260:VAL:HG12	1.87	0.88
2:B:57:ALA:N	2:D:284:ARG:O	2.05	0.88
2:B:398:MET:CG	1:I:348:PRO:HD3	2.03	0.88
1:A:176:GLN:CB	2:B:333:LEU:CD2	2.36	0.88
1:C:176:GLN:CB	2:D:333:LEU:CD2	2.36	0.88
1:E:181:VAL:HA	2:F:352:LYS:HE3	0.91	0.88
1:O:394:LYS:HZ1	2:P:349:ASN:HD21	0.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:404:PHE:HZ	2:R:314:THR:HG22	1.38	0.88
1:A:258:ASN:C	2:P:404:PHE:CE2	2.46	0.88
1:E:97:GLU:OE2	2:F:2:ARG:CZ	2.21	0.88
1:A:100:ALA:CA	2:B:254:LYS:HB2	2.02	0.88
1:C:348:PRO:CD	2:N:398:MET:HG2	2.03	0.88
1:K:394:LYS:HA	2:L:348:PRO:HG3	1.56	0.88
1:E:224:TYR:CG	2:F:325:MET:HG3	2.09	0.88
1:M:407:TRP:CD2	2:N:257:VAL:HA	2.09	0.88
1:Q:101:ASN:N	2:R:254:LYS:CD	2.36	0.88
2:B:56:ALA:CB	2:D:283:TYR:CA	2.51	0.88
1:A:401:LYS:CG	2:B:346:TRP:CG	2.56	0.87
1:E:401:LYS:CE	2:F:346:TRP:CD1	2.55	0.87
1:G:283:HIS:CA	1:I:56:THR:HG21	2.03	0.87
2:J:228:ASN:HD21	5:J:901:GDP:HN1	1.17	0.87
1:M:210:TYR:HB3	2:N:326:LYS:CE	2.03	0.87
1:O:100:ALA:C	2:P:254:LYS:HD2	1.95	0.87
1:A:97:GLU:OE2	2:B:2:ARG:CZ	2.21	0.87
1:C:348:PRO:HD3	2:N:398:MET:HG2	1.56	0.87
1:G:210:TYR:CZ	2:H:326:LYS:N	2.42	0.87
1:K:101:ASN:HB2	2:L:254:LYS:CD	2.03	0.87
1:M:100:ALA:HA	2:N:254:LYS:CB	2.03	0.87
1:C:404:PHE:CE2	2:D:258:ASN:O	2.28	0.87
1:G:224:TYR:CZ	2:H:325:MET:SD	2.66	0.87
1:I:210:TYR:CZ	2:J:326:LYS:CB	2.58	0.87
1:I:224:TYR:CD2	2:J:325:MET:HG3	2.09	0.87
1:K:210:TYR:HB3	2:L:326:LYS:CD	2.03	0.87
1:A:346:TRP:HZ3	2:P:403:ALA:HB1	0.98	0.87
1:M:101:ASN:HB2	2:N:254:LYS:HE3	0.88	0.87
1:M:394:LYS:HZ1	2:N:349:ASN:HD21	0.90	0.87
2:B:403:ALA:HB2	1:I:346:TRP:HE3	1.37	0.87
1:C:401:LYS:HG3	2:D:346:TRP:HB3	1.55	0.87
1:E:407:TRP:CE2	2:F:257:VAL:HA	2.10	0.87
1:G:100:ALA:CA	2:H:254:LYS:HB2	2.03	0.87
1:I:224:TYR:CD1	2:J:325:MET:CG	2.55	0.87
1:M:406:HIS:NE2	2:N:260:VAL:CG1	2.38	0.87
1:Q:176:GLN:HB3	2:R:333:LEU:HD22	0.88	0.87
1:C:401:LYS:HE2	2:D:346:TRP:CD1	2.10	0.87
1:G:404:PHE:H	2:H:261:PRO:CA	1.87	0.87
2:H:283:TYR:C	2:J:56:ALA:CB	2.40	0.87
1:I:210:TYR:HB3	2:J:326:LYS:CE	2.04	0.87
1:K:404:PHE:H	2:L:261:PRO:CA	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:100:ALA:HA	2:R:254:LYS:CB	2.02	0.87
1:Q:177:VAL:HG11	2:R:329:ASP:CA	2.05	0.87
1:C:101:ASN:CG	2:D:254:LYS:HE3	1.95	0.86
1:E:406:HIS:NE2	2:F:260:VAL:HG12	1.90	0.86
2:F:401:ARG:CB	1:K:346:TRP:HB2	2.04	0.86
1:M:177:VAL:HG11	2:N:329:ASP:CA	2.05	0.86
1:Q:101:ASN:HB2	2:R:254:LYS:HE3	0.88	0.86
1:C:210:TYR:HB3	2:D:326:LYS:HD2	1.57	0.86
2:H:284:ARG:O	2:J:57:ALA:N	2.07	0.86
1:M:179:THR:HA	2:N:353:THR:H	1.40	0.86
1:O:176:GLN:HG3	2:P:333:LEU:HD21	1.56	0.86
1:Q:96:LYS:O	2:R:2:ARG:CD	2.23	0.86
1:O:105:ARG:NH2	2:P:253:ARG:HH21	1.58	0.86
1:Q:407:TRP:CD2	2:R:257:VAL:HA	2.10	0.86
1:E:406:HIS:HE1	2:F:260:VAL:O	1.55	0.86
2:F:179:ASP:O	1:K:352:LYS:HA	1.75	0.86
1:G:224:TYR:CZ	2:H:325:MET:CG	2.58	0.86
1:G:407:TRP:CD2	2:H:257:VAL:HA	2.10	0.86
1:K:177:VAL:HG11	2:L:329:ASP:CA	2.06	0.86
1:O:210:TYR:CD1	2:P:326:LYS:CB	2.58	0.86
1:A:2:ARG:CG	2:P:96:GLN:NE2	2.11	0.86
2:B:283:TYR:HA	2:F:56:ALA:HB3	1.57	0.86
1:K:224:TYR:HE1	2:L:325:MET:SD	1.77	0.86
1:M:283:HIS:CA	1:O:56:THR:HG21	2.05	0.86
1:G:177:VAL:HG11	2:H:329:ASP:CA	2.05	0.86
1:I:179:THR:HG21	2:J:353:THR:OG1	1.75	0.86
1:I:394:LYS:HZ1	2:J:349:ASN:HD21	1.20	0.86
1:E:346:TRP:HZ3	2:R:403:ALA:HB1	1.08	0.86
1:E:348:PRO:HD3	2:R:398:MET:HG2	1.56	0.86
1:K:176:GLN:HB3	2:L:333:LEU:HD22	0.86	0.86
1:A:326:LYS:HB2	2:P:210:TYR:CE2	2.09	0.86
1:K:224:TYR:CZ	2:L:325:MET:SD	2.67	0.86
2:B:283:TYR:C	2:F:56:ALA:CB	2.43	0.86
1:M:224:TYR:CE2	2:N:325:MET:HG3	2.07	0.86
1:M:404:PHE:HZ	2:N:314:THR:HG22	1.40	0.86
1:A:224:TYR:HE1	2:B:325:MET:SD	1.88	0.86
1:I:394:LYS:CA	2:J:348:PRO:HG3	2.05	0.86
1:K:224:TYR:CZ	2:L:325:MET:CG	2.58	0.86
1:Q:210:TYR:CZ	2:R:326:LYS:CB	2.58	0.86
2:B:401:ARG:CB	1:I:346:TRP:CB	2.54	0.85
1:C:210:TYR:CE2	2:D:326:LYS:CA	2.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:TYR:CE2	2:H:325:MET:HG3	2.11	0.85
1:G:394:LYS:NZ	2:H:349:ASN:HD21	1.74	0.85
1:K:394:LYS:NZ	2:L:349:ASN:HD21	1.74	0.85
1:A:210:TYR:HB3	2:B:326:LYS:HD2	1.58	0.85
1:C:100:ALA:CA	2:D:254:LYS:HB2	2.05	0.85
1:K:407:TRP:CD2	2:L:257:VAL:HA	2.11	0.85
1:A:224:TYR:CG	2:B:325:MET:HG3	2.11	0.85
2:B:404:PHE:HE2	1:I:258:ASN:C	1.79	0.85
1:M:176:GLN:HB3	2:N:333:LEU:HD22	0.86	0.85
1:Q:406:HIS:NE2	2:R:260:VAL:CG1	2.38	0.85
1:E:96:LYS:NZ	2:F:130:ASP:OD2	2.08	0.85
2:B:398:MET:CG	1:I:348:PRO:CD	2.54	0.85
2:B:401:ARG:CG	1:I:346:TRP:CB	2.39	0.85
1:E:176:GLN:CB	2:F:333:LEU:CD2	2.35	0.85
1:E:404:PHE:H	2:F:261:PRO:CA	1.87	0.85
1:K:210:TYR:HB3	2:L:326:LYS:CE	2.06	0.85
1:K:224:TYR:CD2	2:L:325:MET:HG3	2.12	0.85
1:O:210:TYR:CG	2:P:326:LYS:CG	2.59	0.85
1:A:394:LYS:CA	2:B:348:PRO:HG3	2.07	0.85
1:E:249:ASN:H	2:R:11:GLN:HE22	1.25	0.85
1:O:177:VAL:HG22	2:P:329:ASP:O	1.75	0.85
1:A:401:LYS:HG3	2:B:346:TRP:HB3	1.57	0.85
1:M:97:GLU:CD	2:N:2:ARG:HE	1.79	0.85
2:B:62:VAL:HG22	2:D:283:TYR:CD2	2.11	0.85
1:E:346:TRP:CB	2:R:401:ARG:CG	2.38	0.85
1:O:97:GLU:CD	2:P:2:ARG:CZ	2.43	0.85
1:O:97:GLU:CD	2:P:2:ARG:NE	2.29	0.85
2:P:283:TYR:HB3	2:R:62:VAL:HG21	1.56	0.85
1:C:97:GLU:OE2	2:D:2:ARG:CZ	2.24	0.85
1:A:96:LYS:O	2:B:2:ARG:CD	2.24	0.84
1:K:179:THR:HG21	2:L:353:THR:OG1	1.76	0.84
1:K:210:TYR:CZ	2:L:326:LYS:N	2.45	0.84
2:N:284:ARG:N	2:P:56:ALA:HB1	1.91	0.84
1:C:181:VAL:HA	2:D:352:LYS:HE3	0.87	0.84
2:J:284:ARG:N	2:L:56:ALA:HB1	1.91	0.84
1:K:210:TYR:CZ	2:L:326:LYS:CB	2.60	0.84
1:M:210:TYR:CZ	2:N:326:LYS:CB	2.59	0.84
2:F:96:GLN:HE22	1:K:2:ARG:HG3	0.71	0.84
1:I:238:ILE:O	1:I:238:ILE:HG22	1.77	0.84
1:O:394:LYS:HG2	2:P:348:PRO:CB	2.07	0.84
1:Q:394:LYS:HG2	2:R:348:PRO:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:PRO:CD	2:R:398:MET:HG2	2.07	0.84
2:H:283:TYR:HB3	2:J:62:VAL:HG21	1.57	0.84
1:M:394:LYS:HG2	2:N:348:PRO:CB	2.08	0.84
1:A:238:ILE:O	1:A:238:ILE:HG22	1.78	0.84
1:C:401:LYS:HD3	2:D:346:TRP:CD2	2.12	0.84
1:G:394:LYS:HZ1	2:H:349:ASN:HD21	1.23	0.84
1:K:101:ASN:CG	2:L:254:LYS:HE3	1.98	0.84
1:O:238:ILE:O	1:O:238:ILE:HG22	1.77	0.84
1:A:397:LEU:HB3	2:B:346:TRP:O	1.76	0.84
2:D:181:VAL:HA	1:G:350:GLY:HA3	1.59	0.84
1:E:394:LYS:HA	2:F:348:PRO:HG3	1.60	0.84
1:I:210:TYR:CB	2:J:326:LYS:HD2	2.06	0.84
1:O:210:TYR:CZ	2:P:326:LYS:HB2	2.11	0.84
1:A:210:TYR:CE2	2:B:326:LYS:CA	2.57	0.84
1:A:224:TYR:CZ	2:B:325:MET:HG3	2.11	0.84
1:C:258:ASN:C	2:N:404:PHE:CE2	2.50	0.84
1:C:394:LYS:HZ1	2:D:349:ASN:HD21	1.25	0.84
1:E:100:ALA:CA	2:F:254:LYS:HB2	2.06	0.84
1:M:210:TYR:CB	2:N:326:LYS:HD2	2.08	0.84
1:O:404:PHE:CZ	2:P:314:THR:CG2	2.60	0.84
2:B:96:GLN:HE22	1:I:2:ARG:HG3	0.68	0.84
1:C:224:TYR:HE1	2:D:325:MET:SD	1.90	0.84
1:C:238:ILE:HG22	1:C:238:ILE:O	1.77	0.84
2:J:283:TYR:HA	2:L:56:ALA:HB2	1.60	0.84
1:K:238:ILE:HG22	1:K:238:ILE:O	1.77	0.84
1:M:238:ILE:HG22	1:M:238:ILE:O	1.78	0.84
1:O:404:PHE:HE2	2:P:258:ASN:O	1.57	0.84
1:A:96:LYS:NZ	2:B:130:ASP:OD2	2.11	0.84
1:C:96:LYS:NZ	2:D:130:ASP:OD2	2.10	0.84
1:G:210:TYR:CZ	2:H:326:LYS:CB	2.61	0.84
1:G:224:TYR:CD2	2:H:325:MET:HG3	2.13	0.84
1:G:238:ILE:O	1:G:238:ILE:HG22	1.78	0.83
1:I:101:ASN:N	2:J:254:LYS:CD	2.41	0.83
1:O:101:ASN:HB2	2:P:254:LYS:CG	2.07	0.83
1:Q:176:GLN:HG3	2:R:333:LEU:HD21	1.60	0.83
1:A:181:VAL:HA	2:B:352:LYS:HE3	0.84	0.83
1:K:394:LYS:CA	2:L:348:PRO:HG3	2.08	0.83
1:C:249:ASN:H	2:N:11:GLN:HE22	1.23	0.83
2:D:404:PHE:HE2	1:G:258:ASN:C	1.82	0.83
1:E:101:ASN:HB2	2:F:254:LYS:CD	2.07	0.83
1:G:224:TYR:CD1	2:H:325:MET:CG	2.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:GLN:CG	2:J:333:LEU:HD21	2.07	0.83
1:K:406:HIS:NE2	2:L:260:VAL:HG12	1.93	0.83
1:A:350:GLY:O	2:P:181:VAL:HG23	1.77	0.83
1:E:238:ILE:HG22	1:E:238:ILE:O	1.78	0.83
1:G:179:THR:HG21	2:H:353:THR:OG1	1.79	0.83
1:K:394:LYS:HZ1	2:L:349:ASN:HD21	1.25	0.83
1:O:105:ARG:HH21	2:P:253:ARG:HH21	0.84	0.83
1:Q:238:ILE:O	1:Q:238:ILE:HG22	1.77	0.83
1:M:101:ASN:HB2	2:N:254:LYS:CG	2.09	0.83
1:O:401:LYS:CD	2:P:346:TRP:CD1	2.61	0.83
1:C:326:LYS:HB2	2:N:210:TYR:CE2	2.13	0.83
2:F:403:ALA:HB2	1:K:346:TRP:HE3	1.44	0.83
1:I:394:LYS:HG2	2:J:348:PRO:HB2	1.59	0.83
1:O:101:ASN:HB2	2:P:254:LYS:HE3	0.84	0.83
1:O:401:LYS:HG3	2:P:346:TRP:HB3	1.61	0.83
2:F:181:VAL:HA	1:K:350:GLY:HA3	1.61	0.83
1:K:181:VAL:HA	2:L:352:LYS:HE3	0.84	0.83
1:Q:210:TYR:CD1	2:R:326:LYS:CB	2.60	0.83
1:Q:179:THR:HA	2:R:353:THR:H	1.43	0.83
2:B:398:MET:HG2	1:I:348:PRO:HD3	1.61	0.83
1:G:210:TYR:CB	2:H:326:LYS:HD2	2.08	0.83
1:O:181:VAL:HB	2:P:352:LYS:HG3	1.60	0.83
1:Q:394:LYS:HZ1	2:R:349:ASN:ND2	1.77	0.83
1:A:329:ASN:CG	2:P:177:VAL:CG2	2.46	0.82
1:C:224:TYR:CZ	2:D:325:MET:HG3	2.13	0.82
1:E:224:TYR:CD1	2:F:325:MET:CG	2.61	0.82
1:O:176:GLN:HB3	2:P:333:LEU:CG	2.08	0.82
2:B:56:ALA:CB	2:D:283:TYR:C	2.48	0.82
1:C:401:LYS:CE	2:D:346:TRP:CD1	2.61	0.82
1:G:176:GLN:HB3	2:H:333:LEU:HD22	0.83	0.82
1:C:224:TYR:CG	2:D:325:MET:HG3	2.13	0.82
2:D:401:ARG:CG	1:G:346:TRP:CB	2.43	0.82
1:G:394:LYS:CA	2:H:348:PRO:HG3	2.09	0.82
1:M:101:ASN:H	2:N:254:LYS:HD2	1.42	0.82
1:O:210:TYR:CD2	2:P:326:LYS:CG	2.62	0.82
2:D:96:GLN:HE22	1:G:2:ARG:HG3	0.66	0.82
1:E:404:PHE:CE2	2:F:258:ASN:O	2.32	0.82
1:G:210:TYR:HB3	2:H:326:LYS:CE	2.08	0.82
1:K:224:TYR:CE2	2:L:325:MET:HG3	2.13	0.82
2:P:282:GLN:O	2:R:60:LYS:HB2	1.78	0.82
1:C:2:ARG:CG	2:N:96:GLN:NE2	2.17	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:MET:CG	1:G:348:PRO:HD3	2.09	0.82
1:E:401:LYS:NZ	2:F:437:ASP:OD2	2.11	0.82
1:I:406:HIS:NE2	2:J:260:VAL:HG12	1.94	0.82
1:K:176:GLN:CG	2:L:333:LEU:HD21	2.10	0.82
1:Q:101:ASN:CB	2:R:254:LYS:CE	2.31	0.82
1:Q:210:TYR:CG	2:R:326:LYS:CG	2.62	0.82
1:A:210:TYR:CE1	2:B:326:LYS:CB	2.62	0.82
1:E:224:TYR:CZ	2:F:325:MET:HG3	2.14	0.82
1:I:176:GLN:HB3	2:J:333:LEU:HD22	0.82	0.82
1:I:210:TYR:CZ	2:J:326:LYS:HB2	2.14	0.82
2:B:210:TYR:CE2	1:I:326:LYS:HB2	2.14	0.82
1:O:101:ASN:H	2:P:254:LYS:HD2	1.39	0.82
1:O:177:VAL:CG1	2:P:329:ASP:HA	2.08	0.82
1:O:401:LYS:CE	2:P:346:TRP:CD1	2.63	0.82
1:K:101:ASN:HB2	2:L:254:LYS:HE3	0.82	0.82
2:F:398:MET:CG	1:K:348:PRO:HD3	2.09	0.81
1:A:256:GLN:HG2	2:P:407:TRP:CH2	2.15	0.81
1:G:406:HIS:NE2	2:H:260:VAL:HG12	1.95	0.81
1:K:404:PHE:HZ	2:L:314:THR:HG22	1.45	0.81
1:O:210:TYR:CG	2:P:326:LYS:HG3	2.15	0.81
1:G:101:ASN:HB2	2:H:254:LYS:HE3	0.81	0.81
1:I:397:LEU:HB3	2:J:346:TRP:O	1.80	0.81
1:O:210:TYR:OH	2:P:325:MET:C	2.17	0.81
1:Q:101:ASN:H	2:R:254:LYS:HD2	1.42	0.81
1:C:394:LYS:CA	2:D:348:PRO:HG3	2.09	0.81
1:C:397:LEU:HB3	2:D:346:TRP:O	1.81	0.81
1:I:394:LYS:NZ	2:J:349:ASN:ND2	2.29	0.81
1:M:210:TYR:CG	2:N:326:LYS:CG	2.63	0.81
1:M:404:PHE:HE2	2:N:258:ASN:O	1.63	0.81
2:B:398:MET:HG2	1:I:348:PRO:CD	2.10	0.81
1:C:406:HIS:NE2	2:D:260:VAL:HG12	1.95	0.81
1:K:176:GLN:HB2	2:L:333:LEU:HD22	1.59	0.81
1:M:100:ALA:C	2:N:254:LYS:HD2	2.01	0.81
1:A:210:TYR:OH	2:B:326:LYS:N	2.13	0.81
1:G:176:GLN:CG	2:H:333:LEU:HD21	2.11	0.81
1:I:176:GLN:HB2	2:J:333:LEU:HD22	1.59	0.81
1:M:176:GLN:CG	2:N:333:LEU:CD2	2.57	0.81
1:M:176:GLN:HG3	2:N:333:LEU:HD21	1.61	0.81
1:Q:210:TYR:CG	2:R:326:LYS:HG3	2.15	0.81
1:A:401:LYS:HE2	2:B:346:TRP:CD1	2.15	0.81
2:B:284:ARG:N	2:F:56:ALA:HB1	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:CD2	2:B:257:VAL:HA	2.16	0.81
1:Q:176:GLN:CG	2:R:333:LEU:CD2	2.58	0.81
1:I:100:ALA:C	2:J:254:LYS:HD2	2.00	0.81
2:N:283:TYR:HB3	2:P:62:VAL:HG21	1.60	0.81
1:Q:11:GLN:CD	2:R:247:GLN:O	2.18	0.81
1:A:133:GLN:HE22	2:P:97:SER:CB	1.93	0.81
1:A:394:LYS:HG2	2:B:348:PRO:HB2	1.61	0.81
1:C:210:TYR:CE1	2:D:326:LYS:CB	2.64	0.80
1:G:181:VAL:HA	2:H:352:LYS:HE3	0.82	0.80
1:E:2:ARG:CG	2:R:96:GLN:NE2	2.20	0.80
1:G:394:LYS:HG2	2:H:348:PRO:HB2	1.63	0.80
1:G:401:LYS:CD	2:H:346:TRP:CG	2.65	0.80
1:I:404:PHE:HE2	2:J:258:ASN:O	1.61	0.80
1:K:394:LYS:HG2	2:L:348:PRO:HB2	1.62	0.80
1:M:179:THR:CG2	2:N:353:THR:HG1	1.87	0.80
1:Q:210:TYR:CB	2:R:326:LYS:HD2	2.10	0.80
1:Q:401:LYS:CE	2:R:346:TRP:CD1	2.65	0.80
1:C:96:LYS:O	2:D:2:ARG:CD	2.28	0.80
2:D:210:TYR:CE2	1:G:326:LYS:HB2	2.17	0.80
1:A:224:TYR:CZ	2:B:325:MET:SD	2.73	0.80
1:G:210:TYR:CZ	2:H:326:LYS:HB2	2.16	0.80
1:M:96:LYS:NZ	2:N:130:ASP:OD2	2.13	0.80
1:G:404:PHE:HE2	2:H:258:ASN:O	1.63	0.80
1:I:96:LYS:O	2:J:2:ARG:CD	2.29	0.80
1:I:404:PHE:HZ	2:J:314:THR:HG22	1.46	0.80
2:J:282:GLN:O	2:L:60:LYS:HB2	1.80	0.80
1:I:101:ASN:CB	2:J:254:LYS:CE	2.28	0.80
1:I:179:THR:HA	2:J:353:THR:H	1.47	0.80
1:Q:401:LYS:HE2	2:R:346:TRP:CD1	2.17	0.80
1:A:247:ALA:O	2:P:11:GLN:OE1	1.98	0.80
1:I:101:ASN:HB2	2:J:254:LYS:HE3	0.81	0.80
1:A:401:LYS:HD3	2:B:346:TRP:CD2	2.17	0.80
1:A:406:HIS:NE2	2:B:260:VAL:HG12	1.96	0.80
1:K:401:LYS:NZ	2:L:437:ASP:OD2	2.14	0.80
1:K:404:PHE:HZ	2:L:314:THR:CG2	1.94	0.80
1:M:401:LYS:HG3	2:N:346:TRP:HB3	1.63	0.80
2:D:398:MET:CG	1:G:348:PRO:CD	2.60	0.80
1:M:97:GLU:CD	2:N:2:ARG:CZ	2.49	0.80
1:O:11:GLN:CD	2:P:247:GLN:O	2.20	0.80
1:A:210:TYR:HB3	2:B:326:LYS:CD	2.12	0.80
1:E:101:ASN:CG	2:F:254:LYS:HE3	2.03	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:TYR:HB3	2:F:326:LYS:HD2	1.63	0.80
1:M:404:PHE:CZ	2:N:314:THR:CG2	2.64	0.80
1:O:105:ARG:CZ	2:P:253:ARG:NE	2.45	0.80
1:O:406:HIS:CE1	2:P:260:VAL:CG1	2.65	0.80
1:Q:97:GLU:CD	2:R:2:ARG:HE	1.83	0.80
1:Q:176:GLN:HB3	2:R:333:LEU:CG	2.10	0.80
1:A:210:TYR:CZ	2:B:326:LYS:N	2.50	0.79
1:E:326:LYS:HB2	2:R:210:TYR:CE2	2.16	0.79
1:E:329:ASN:OD1	2:R:177:VAL:HG21	1.82	0.79
1:G:401:LYS:CG	2:H:346:TRP:HB3	2.12	0.79
1:A:394:LYS:NZ	2:B:349:ASN:HD21	1.80	0.79
2:B:56:ALA:HB3	2:D:283:TYR:HA	1.62	0.79
1:E:133:GLN:HE22	2:R:97:SER:CB	1.95	0.79
1:M:210:TYR:OH	2:N:325:MET:C	2.21	0.79
1:O:179:THR:CA	2:P:353:THR:H	1.96	0.79
1:Q:179:THR:O	2:R:352:LYS:HB3	1.82	0.79
1:A:224:TYR:CD1	2:B:325:MET:CG	2.64	0.79
1:C:210:TYR:OH	2:D:326:LYS:N	2.15	0.79
1:K:210:TYR:CZ	2:L:326:LYS:HB2	2.17	0.79
1:O:404:PHE:CZ	2:P:314:THR:HG21	2.17	0.79
1:O:407:TRP:CZ2	2:P:256:ALA:O	2.35	0.79
1:Q:404:PHE:CZ	2:R:314:THR:CG2	2.64	0.79
1:A:258:ASN:O	2:P:404:PHE:CZ	2.35	0.79
1:C:394:LYS:HG2	2:D:348:PRO:HB2	1.64	0.79
1:E:179:THR:HG21	2:F:353:THR:OG1	1.82	0.79
1:I:97:GLU:CD	2:J:2:ARG:HE	1.85	0.79
1:I:210:TYR:CG	2:J:326:LYS:CG	2.65	0.79
1:K:101:ASN:N	2:L:254:LYS:CD	2.44	0.79
1:M:210:TYR:CG	2:N:326:LYS:HG3	2.18	0.79
1:O:176:GLN:HB3	2:P:333:LEU:HD22	0.80	0.79
1:C:210:TYR:HB3	2:D:326:LYS:CD	2.12	0.79
1:C:407:TRP:CD2	2:D:257:VAL:HA	2.18	0.79
1:G:176:GLN:HB2	2:H:333:LEU:HD22	1.63	0.79
1:O:179:THR:HB	2:P:353:THR:O	1.82	0.79
2:D:401:ARG:CB	1:G:346:TRP:CB	2.61	0.79
2:H:284:ARG:N	2:J:56:ALA:HB1	1.96	0.79
1:M:401:LYS:CE	2:N:346:TRP:CD1	2.66	0.79
1:O:177:VAL:HG21	2:P:329:ASP:CA	2.12	0.79
1:Q:96:LYS:NZ	2:R:130:ASP:OD2	2.15	0.79
1:E:210:TYR:CE1	2:F:326:LYS:CB	2.63	0.79
1:E:258:ASN:C	2:R:404:PHE:CE2	2.56	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:210:TYR:CE2	1:K:326:LYS:HB2	2.17	0.79
1:O:101:ASN:CA	2:P:254:LYS:HE3	2.13	0.79
1:O:398:MET:HG3	2:P:348:PRO:HD2	1.65	0.79
1:Q:210:TYR:CZ	2:R:326:LYS:HB2	2.18	0.79
1:Q:401:LYS:NZ	2:R:437:ASP:OD2	2.15	0.79
2:B:283:TYR:HB3	2:F:62:VAL:HG21	1.65	0.79
2:N:345:GLU:OE1	2:N:345:GLU:N	2.16	0.79
1:Q:404:PHE:HE2	2:R:258:ASN:O	1.66	0.79
1:C:224:TYR:CZ	2:D:325:MET:SD	2.75	0.79
1:I:401:LYS:CD	2:J:346:TRP:CG	2.66	0.79
1:I:404:PHE:HZ	2:J:314:THR:CG2	1.94	0.79
2:F:401:ARG:HG3	1:K:346:TRP:HB3	0.86	0.79
1:I:181:VAL:HA	2:J:352:LYS:HE3	0.79	0.79
1:K:11:GLN:CD	2:L:247:GLN:O	2.21	0.79
1:M:97:GLU:CD	2:N:2:ARG:NE	2.35	0.79
1:M:176:GLN:HB3	2:N:333:LEU:CG	2.12	0.79
1:Q:100:ALA:C	2:R:254:LYS:HD2	2.03	0.79
1:E:394:LYS:CA	2:F:348:PRO:HG3	2.13	0.78
2:F:404:PHE:HE2	1:K:258:ASN:C	1.86	0.78
1:A:401:LYS:CE	2:B:346:TRP:CD1	2.66	0.78
2:B:11:GLN:HE22	1:I:249:ASN:H	1.30	0.78
1:G:101:ASN:N	2:H:254:LYS:CD	2.44	0.78
2:J:345:GLU:OE1	2:J:345:GLU:N	2.16	0.78
1:M:177:VAL:HG22	2:N:329:ASP:O	1.83	0.78
1:A:179:THR:HG21	2:B:353:THR:OG1	1.81	0.78
2:B:345:GLU:OE1	2:B:345:GLU:N	2.16	0.78
1:E:210:TYR:OH	2:F:326:LYS:N	2.16	0.78
1:I:176:GLN:CG	2:J:333:LEU:CD2	2.62	0.78
1:Q:401:LYS:CD	2:R:346:TRP:CD1	2.66	0.78
1:K:100:ALA:HA	2:L:254:LYS:CB	2.11	0.78
1:Q:101:ASN:HB2	2:R:254:LYS:CG	2.13	0.78
1:C:179:THR:HG21	2:D:353:THR:OG1	1.83	0.78
1:E:404:PHE:HZ	2:F:314:THR:HG22	1.47	0.78
1:G:404:PHE:HZ	2:H:314:THR:CG2	1.97	0.78
1:M:11:GLN:CD	2:N:247:GLN:O	2.22	0.78
1:O:401:LYS:HD3	2:P:346:TRP:CD1	2.17	0.78
2:P:345:GLU:OE1	2:P:345:GLU:N	2.16	0.78
1:Q:97:GLU:CD	2:R:2:ARG:CZ	2.50	0.78
1:C:224:TYR:CD1	2:D:325:MET:CG	2.66	0.78
1:C:256:GLN:HG2	2:N:407:TRP:CH2	2.17	0.78
1:G:101:ASN:CB	2:H:254:LYS:CE	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LYS:CD	2:J:346:TRP:CD1	2.67	0.78
1:K:181:VAL:HA	2:L:352:LYS:NZ	1.98	0.78
1:O:210:TYR:CG	2:P:326:LYS:HD2	2.19	0.78
1:A:404:PHE:HZ	2:B:314:THR:CG2	1.96	0.78
1:E:247:ALA:O	2:R:11:GLN:OE1	2.00	0.78
1:G:401:LYS:CD	2:H:346:TRP:CD1	2.66	0.78
1:Q:401:LYS:HG3	2:R:346:TRP:HB3	1.64	0.78
1:E:407:TRP:CD2	2:F:257:VAL:HA	2.18	0.78
1:G:397:LEU:HB3	2:H:346:TRP:O	1.84	0.78
1:I:401:LYS:CG	2:J:346:TRP:HB3	2.13	0.78
1:O:401:LYS:HE2	2:P:346:TRP:CD1	2.19	0.78
2:P:283:TYR:HB3	2:R:62:VAL:CG2	2.14	0.78
2:F:398:MET:CG	1:K:348:PRO:CD	2.61	0.78
1:G:181:VAL:HA	2:H:352:LYS:NZ	1.98	0.78
1:K:210:TYR:CB	2:L:326:LYS:HD2	2.13	0.78
1:C:404:PHE:HZ	2:D:314:THR:CG2	1.97	0.77
1:M:401:LYS:CD	2:N:346:TRP:CD1	2.67	0.77
2:D:403:ALA:HB2	1:G:346:TRP:HE3	1.44	0.77
1:E:96:LYS:O	2:F:2:ARG:CD	2.31	0.77
1:G:100:ALA:C	2:H:254:LYS:HD2	2.03	0.77
2:L:345:GLU:OE1	2:L:345:GLU:N	2.16	0.77
1:O:401:LYS:HD3	2:P:346:TRP:CD2	2.19	0.77
1:G:96:LYS:O	2:H:2:ARG:CD	2.32	0.77
1:G:394:LYS:NZ	2:H:349:ASN:ND2	2.32	0.77
1:I:181:VAL:HA	2:J:352:LYS:NZ	1.98	0.77
2:J:283:TYR:HB3	2:L:62:VAL:CG2	2.13	0.77
1:M:210:TYR:CZ	2:N:326:LYS:HB2	2.18	0.77
2:B:56:ALA:HB1	2:D:284:ARG:N	1.99	0.77
1:C:394:LYS:NZ	2:D:349:ASN:HD21	1.82	0.77
1:K:401:LYS:CD	2:L:346:TRP:CD1	2.68	0.77
1:A:101:ASN:CB	2:B:254:LYS:CE	2.35	0.77
1:C:133:GLN:HE22	2:N:97:SER:CB	1.96	0.77
1:C:210:TYR:CZ	2:D:326:LYS:N	2.51	0.77
2:F:345:GLU:OE1	2:F:345:GLU:N	2.16	0.77
1:G:181:VAL:CB	2:H:352:LYS:CE	2.55	0.77
1:K:394:LYS:NZ	2:L:349:ASN:ND2	2.33	0.77
1:M:210:TYR:CD1	2:N:326:LYS:CB	2.61	0.77
1:O:96:LYS:NZ	2:P:130:ASP:OD2	2.18	0.77
1:A:97:GLU:CD	2:B:2:ARG:HE	1.86	0.77
1:I:11:GLN:CD	2:J:247:GLN:O	2.23	0.77
1:Q:210:TYR:OH	2:R:325:MET:C	2.22	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:CD2	2:B:325:MET:HG3	2.19	0.77
2:B:404:PHE:CE2	1:I:258:ASN:C	2.58	0.77
1:I:97:GLU:CD	2:J:2:ARG:CZ	2.51	0.77
1:A:224:TYR:CZ	2:B:325:MET:CG	2.68	0.77
1:K:100:ALA:C	2:L:254:LYS:HD2	2.04	0.77
1:K:210:TYR:CD1	2:L:326:LYS:CB	2.66	0.77
2:R:345:GLU:OE1	2:R:345:GLU:N	2.16	0.77
1:O:181:VAL:HA	2:P:352:LYS:NZ	2.00	0.77
1:A:101:ASN:HB2	2:B:254:LYS:CG	2.16	0.76
1:I:401:LYS:NZ	2:J:437:ASP:OD2	2.18	0.76
1:M:105:ARG:CZ	2:N:253:ARG:NE	2.48	0.76
1:C:247:ALA:O	2:N:11:GLN:OE1	2.03	0.76
1:E:404:PHE:HZ	2:F:314:THR:CG2	1.97	0.76
1:G:179:THR:HA	2:H:353:THR:H	1.50	0.76
1:I:210:TYR:CD2	2:J:326:LYS:CG	2.67	0.76
1:K:397:LEU:HB3	2:L:346:TRP:O	1.85	0.76
2:D:398:MET:HG2	1:G:348:PRO:HD3	1.67	0.76
1:I:177:VAL:HG22	2:J:329:ASP:O	1.83	0.76
1:M:401:LYS:HE2	2:N:346:TRP:CD1	2.20	0.76
1:K:96:LYS:O	2:L:2:ARG:CD	2.33	0.76
1:A:249:ASN:H	2:P:11:GLN:NE2	1.83	0.76
1:E:177:VAL:HG11	2:F:329:ASP:CA	2.15	0.76
2:F:401:ARG:CB	1:K:346:TRP:CB	2.64	0.76
1:G:404:PHE:HZ	2:H:314:THR:HG22	1.48	0.76
1:I:97:GLU:CD	2:J:2:ARG:NE	2.39	0.76
1:K:210:TYR:CG	2:L:326:LYS:CG	2.68	0.76
1:M:179:THR:HB	2:N:353:THR:O	1.84	0.76
1:C:329:ASN:CG	2:N:177:VAL:CG2	2.52	0.76
1:G:100:ALA:HA	2:H:254:LYS:CB	2.14	0.76
1:G:177:VAL:HG22	2:H:329:ASP:O	1.85	0.76
1:G:401:LYS:NZ	2:H:437:ASP:OD2	2.17	0.76
1:M:210:TYR:CD2	2:N:326:LYS:CG	2.69	0.76
1:O:101:ASN:HD22	2:P:258:ASN:HD21	1.34	0.76
1:A:177:VAL:HG11	2:B:329:ASP:CA	2.16	0.76
1:C:258:ASN:O	2:N:404:PHE:CZ	2.38	0.76
1:E:224:TYR:CZ	2:F:325:MET:SD	2.77	0.76
1:K:401:LYS:CD	2:L:346:TRP:CG	2.68	0.76
1:M:181:VAL:HB	2:N:352:LYS:HG3	1.67	0.76
2:N:282:GLN:O	2:P:60:LYS:HB2	1.85	0.76
1:O:11:GLN:OE1	2:P:247:GLN:O	2.04	0.76
1:Q:177:VAL:HG22	2:R:329:ASP:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:GLY:O	2:R:181:VAL:HG23	1.83	0.76
1:A:179:THR:HA	2:B:353:THR:H	1.51	0.76
1:C:350:GLY:O	2:N:181:VAL:HG23	1.82	0.76
1:K:404:PHE:HE2	2:L:258:ASN:O	1.65	0.76
1:Q:97:GLU:CD	2:R:2:ARG:NE	2.38	0.76
1:E:100:ALA:HA	2:F:254:LYS:CB	2.11	0.76
1:E:394:LYS:NZ	2:F:349:ASN:HD21	1.84	0.76
1:M:401:LYS:HD3	2:N:346:TRP:CD2	2.21	0.76
1:C:101:ASN:CB	2:D:254:LYS:CE	2.38	0.75
2:F:11:GLN:HE22	1:K:249:ASN:H	1.34	0.75
1:K:181:VAL:CB	2:L:352:LYS:CE	2.55	0.75
1:O:401:LYS:CG	2:P:346:TRP:CB	2.62	0.75
1:Q:210:TYR:CD2	2:R:326:LYS:CG	2.69	0.75
1:A:224:TYR:CE2	2:B:325:MET:HG3	2.20	0.75
1:I:210:TYR:CG	2:J:326:LYS:HG3	2.21	0.75
1:O:401:LYS:NZ	2:P:437:ASP:OD2	2.18	0.75
1:O:397:LEU:HD22	2:P:345:GLU:O	1.85	0.75
1:C:224:TYR:CD2	2:D:325:MET:HG3	2.22	0.75
1:G:210:TYR:CG	2:H:326:LYS:CG	2.69	0.75
1:I:176:GLN:HG3	2:J:333:LEU:HD21	1.68	0.75
1:I:210:TYR:OH	2:J:325:MET:C	2.24	0.75
1:A:329:ASN:CB	2:P:177:VAL:HG21	2.17	0.75
1:A:394:LYS:NZ	2:B:349:ASN:ND2	2.34	0.75
1:G:176:GLN:CG	2:H:333:LEU:CD2	2.65	0.75
1:K:11:GLN:OE1	2:L:247:GLN:O	2.05	0.75
1:K:97:GLU:CD	2:L:2:ARG:CZ	2.53	0.75
1:Q:105:ARG:CZ	2:R:253:ARG:NE	2.50	0.75
1:Q:401:LYS:HD3	2:R:346:TRP:CD2	2.21	0.75
1:A:404:PHE:HE2	2:B:258:ASN:O	1.68	0.75
2:D:404:PHE:CE2	1:G:258:ASN:C	2.59	0.75
1:G:97:GLU:CD	2:H:2:ARG:HE	1.90	0.75
1:M:401:LYS:NZ	2:N:437:ASP:OD2	2.19	0.75
1:M:404:PHE:CZ	2:N:314:THR:HG21	2.21	0.75
1:O:179:THR:O	2:P:352:LYS:HB3	1.87	0.75
1:M:177:VAL:CG1	2:N:329:ASP:HA	2.15	0.75
1:M:179:THR:O	2:N:352:LYS:HB3	1.86	0.75
1:O:401:LYS:HD3	2:P:346:TRP:NE1	2.00	0.75
1:A:101:ASN:N	2:B:254:LYS:CD	2.46	0.75
2:D:398:MET:HG2	1:G:348:PRO:CD	2.17	0.75
1:E:243:ARG:NH2	2:R:71:GLU:OE2	2.20	0.75
1:I:210:TYR:CG	2:J:326:LYS:HD2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:179:THR:CA	2:N:353:THR:H	1.99	0.75
1:A:406:HIS:NE2	2:B:260:VAL:CG1	2.50	0.75
1:C:177:VAL:HG11	2:D:329:ASP:CA	2.17	0.75
1:E:210:TYR:CZ	2:F:326:LYS:N	2.55	0.75
2:H:283:TYR:HA	2:J:56:ALA:HB2	1.68	0.75
1:K:401:LYS:CG	2:L:346:TRP:HB3	2.17	0.75
1:E:406:HIS:NE2	2:F:260:VAL:CG1	2.49	0.74
2:B:283:TYR:CA	2:F:56:ALA:HB1	2.15	0.74
2:D:11:GLN:HE22	1:G:249:ASN:H	1.32	0.74
2:D:401:ARG:HG3	1:G:346:TRP:HB3	0.81	0.74
1:E:224:TYR:CD2	2:F:325:MET:HG3	2.22	0.74
2:F:398:MET:HG2	1:K:348:PRO:HD3	1.68	0.74
1:K:210:TYR:CG	2:L:326:LYS:HG3	2.22	0.74
1:Q:181:VAL:HA	2:R:352:LYS:NZ	2.02	0.74
1:I:181:VAL:CB	2:J:352:LYS:CE	2.55	0.74
1:Q:11:GLN:OE1	2:R:247:GLN:O	2.05	0.74
1:Q:404:PHE:CZ	2:R:314:THR:HG21	2.22	0.74
1:E:2:ARG:HG3	2:R:96:GLN:HE22	0.62	0.74
2:F:401:ARG:CG	1:K:346:TRP:CB	2.48	0.74
1:I:11:GLN:OE1	2:J:247:GLN:O	2.06	0.74
1:I:177:VAL:HG21	2:J:329:ASP:CA	2.18	0.74
1:O:401:LYS:CG	2:P:346:TRP:HB3	2.17	0.74
1:Q:398:MET:HG3	2:R:348:PRO:HD2	1.69	0.74
1:A:100:ALA:HA	2:B:254:LYS:CB	2.13	0.74
1:C:224:TYR:CZ	2:D:325:MET:CG	2.70	0.74
1:M:177:VAL:HG21	2:N:329:ASP:CA	2.17	0.74
1:O:105:ARG:CZ	2:P:253:ARG:HE	1.99	0.74
1:Q:401:LYS:HD3	2:R:346:TRP:NE1	2.03	0.74
1:C:101:ASN:N	2:D:254:LYS:CD	2.49	0.74
1:C:224:TYR:CE2	2:D:325:MET:HG3	2.22	0.74
1:C:404:PHE:HE2	2:D:258:ASN:O	1.70	0.74
1:E:210:TYR:CE2	2:F:326:LYS:CA	2.61	0.74
1:E:394:LYS:HG2	2:F:348:PRO:HB2	1.68	0.74
1:I:100:ALA:HA	2:J:254:LYS:CB	2.11	0.74
1:I:181:VAL:HB	2:J:352:LYS:HG3	1.69	0.74
1:O:397:LEU:HB3	2:P:346:TRP:C	2.07	0.74
1:C:401:LYS:NZ	2:D:437:ASP:OD2	2.20	0.74
1:E:210:TYR:HB3	2:F:326:LYS:CD	2.16	0.74
1:G:11:GLN:CD	2:H:247:GLN:O	2.26	0.74
1:G:177:VAL:HG21	2:H:329:ASP:CA	2.18	0.74
1:I:210:TYR:CD1	2:J:326:LYS:CB	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:406:HIS:NE2	2:J:260:VAL:CG1	2.50	0.74
1:I:407:TRP:CZ2	2:J:256:ALA:O	2.41	0.74
1:Q:179:THR:CA	2:R:353:THR:H	2.01	0.74
1:A:348:PRO:CG	2:P:398:MET:SD	2.75	0.74
1:K:179:THR:HA	2:L:353:THR:H	1.53	0.74
1:M:407:TRP:CZ2	2:N:256:ALA:O	2.41	0.74
1:A:348:PRO:HD3	2:P:398:MET:HG3	1.68	0.74
1:C:404:PHE:HZ	2:D:314:THR:HG22	1.51	0.74
1:I:177:VAL:CG1	2:J:329:ASP:HA	2.15	0.74
1:K:176:GLN:CG	2:L:333:LEU:CD2	2.66	0.74
1:O:401:LYS:CD	2:P:346:TRP:CG	2.70	0.74
1:Q:179:THR:HB	2:R:353:THR:O	1.88	0.74
1:M:101:ASN:CA	2:N:254:LYS:HE3	2.18	0.73
1:Q:101:ASN:CA	2:R:254:LYS:HE3	2.18	0.73
2:H:282:GLN:O	2:J:60:LYS:HB2	1.88	0.73
1:O:397:LEU:CB	2:P:346:TRP:O	2.36	0.73
1:C:101:ASN:HB2	2:D:254:LYS:CG	2.19	0.73
1:E:224:TYR:CZ	2:F:325:MET:CG	2.71	0.73
1:I:398:MET:HG3	2:J:348:PRO:HD2	1.69	0.73
1:Q:407:TRP:CZ2	2:R:256:ALA:O	2.41	0.73
1:C:406:HIS:NE2	2:D:260:VAL:CG1	2.51	0.73
1:E:401:LYS:CD	2:F:346:TRP:CG	2.71	0.73
1:G:210:TYR:CD2	2:H:326:LYS:CG	2.70	0.73
2:J:266:HIS:ND1	2:J:266:HIS:O	2.22	0.73
1:E:329:ASN:CG	2:R:177:VAL:CG2	2.56	0.73
1:G:398:MET:HG3	2:H:348:PRO:HD2	1.70	0.73
1:K:97:GLU:CD	2:L:2:ARG:HE	1.91	0.73
1:K:406:HIS:NE2	2:L:260:VAL:CG1	2.50	0.73
1:O:176:GLN:OE1	2:P:333:LEU:CD1	2.31	0.73
1:O:181:VAL:HG23	2:P:352:LYS:HE2	1.70	0.73
1:A:404:PHE:HZ	2:B:314:THR:HG22	1.51	0.73
2:B:266:HIS:ND1	2:B:266:HIS:O	2.22	0.73
1:E:101:ASN:N	2:F:254:LYS:CD	2.50	0.73
1:E:401:LYS:CD	2:F:346:TRP:CD1	2.71	0.73
1:I:176:GLN:HB3	2:J:333:LEU:CG	2.18	0.73
1:A:350:GLY:CA	2:P:181:VAL:HA	2.15	0.73
2:B:62:VAL:HG21	2:D:283:TYR:HB3	1.70	0.73
1:E:181:VAL:HA	2:F:352:LYS:NZ	2.03	0.73
2:J:283:TYR:CA	2:L:56:ALA:HB2	2.15	0.73
1:O:100:ALA:HB1	2:P:254:LYS:HA	1.69	0.73
2:P:266:HIS:ND1	2:P:266:HIS:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:345:GLU:OE1	2:H:345:GLU:N	2.16	0.73
1:K:179:THR:HG22	2:L:353:THR:HG1	1.52	0.73
2:P:282:GLN:O	2:R:60:LYS:CB	2.35	0.73
2:B:97:SER:CB	1:I:133:GLN:HE22	2.01	0.73
1:K:398:MET:HG3	2:L:348:PRO:HD2	1.71	0.73
1:O:181:VAL:CB	2:P:352:LYS:CE	2.58	0.73
1:C:100:ALA:HA	2:D:254:LYS:CB	2.14	0.73
1:E:394:LYS:HZ1	2:F:349:ASN:HD21	1.37	0.73
1:K:176:GLN:HG3	2:L:333:LEU:HD21	1.70	0.73
1:K:407:TRP:CZ2	2:L:256:ALA:O	2.42	0.73
1:Q:224:TYR:CE2	2:R:325:MET:HG3	2.09	0.73
1:E:397:LEU:HB3	2:F:346:TRP:O	1.89	0.72
2:F:398:MET:HG2	1:K:348:PRO:CD	2.19	0.72
1:K:177:VAL:HG22	2:L:329:ASP:O	1.88	0.72
1:M:398:MET:HG3	2:N:348:PRO:HD2	1.70	0.72
1:Q:181:VAL:HA	2:R:352:LYS:HE3	0.73	0.72
1:A:329:ASN:OD1	2:P:177:VAL:HG21	1.84	0.72
2:D:345:GLU:OE1	2:D:345:GLU:N	2.16	0.72
2:N:266:HIS:ND1	2:N:266:HIS:O	2.22	0.72
1:Q:176:GLN:HB3	2:R:333:LEU:CD1	2.18	0.72
2:D:266:HIS:ND1	2:D:266:HIS:O	2.22	0.72
1:G:210:TYR:CD1	2:H:326:LYS:CB	2.68	0.72
2:H:266:HIS:ND1	2:H:266:HIS:O	2.22	0.72
1:I:96:LYS:NZ	2:J:130:ASP:OD2	2.22	0.72
1:I:101:ASN:H	2:J:254:LYS:HD2	1.51	0.72
1:I:105:ARG:NH2	2:J:253:ARG:HH21	1.66	0.72
1:K:101:ASN:H	2:L:254:LYS:HD2	1.53	0.72
2:N:283:TYR:HB3	2:P:62:VAL:CG2	2.18	0.72
1:C:179:THR:HA	2:D:353:THR:H	1.53	0.72
1:G:407:TRP:CZ2	2:H:256:ALA:O	2.43	0.72
1:I:101:ASN:HB2	2:J:254:LYS:CG	2.19	0.72
1:M:11:GLN:OE1	2:N:247:GLN:O	2.08	0.72
1:M:101:ASN:HD22	2:N:258:ASN:HD21	1.37	0.72
1:O:101:ASN:CA	2:P:254:LYS:CE	2.68	0.72
1:A:100:ALA:C	2:B:254:LYS:HD2	2.09	0.72
1:C:394:LYS:NZ	2:D:349:ASN:ND2	2.36	0.72
1:E:348:PRO:HD3	2:R:398:MET:HG3	1.71	0.72
2:F:96:GLN:NE2	1:K:2:ARG:CG	2.33	0.72
1:G:406:HIS:NE2	2:H:260:VAL:CG1	2.52	0.72
2:L:266:HIS:ND1	2:L:266:HIS:O	2.22	0.72
1:E:11:GLN:CD	2:F:247:GLN:O	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:LYS:NZ	2:H:130:ASP:OD2	2.21	0.72
2:H:283:TYR:HB3	2:J:62:VAL:CG2	2.19	0.72
1:M:407:TRP:NE1	2:N:260:VAL:HB	2.05	0.72
1:Q:105:ARG:NH2	2:R:253:ARG:NE	2.37	0.72
1:Q:181:VAL:CB	2:R:352:LYS:CE	2.61	0.72
1:A:256:GLN:O	2:P:407:TRP:CZ2	2.42	0.72
1:O:179:THR:CG2	2:P:353:THR:HG1	2.02	0.72
2:F:71:GLU:OE2	1:K:243:ARG:NH2	2.23	0.72
1:G:181:VAL:HB	2:H:352:LYS:HG3	1.72	0.72
1:G:210:TYR:CG	2:H:326:LYS:HD2	2.24	0.72
1:K:101:ASN:CB	2:L:254:LYS:CE	2.34	0.72
2:D:97:SER:CB	1:G:133:GLN:HE22	2.02	0.72
1:M:105:ARG:CZ	2:N:253:ARG:HE	2.03	0.72
1:C:97:GLU:CD	2:D:2:ARG:HE	1.92	0.71
1:O:105:ARG:NH2	2:P:253:ARG:NE	2.38	0.71
1:O:210:TYR:CG	2:P:326:LYS:HB2	2.26	0.71
1:Q:181:VAL:HB	2:R:352:LYS:HG3	1.70	0.71
1:Q:210:TYR:CG	2:R:326:LYS:HD2	2.25	0.71
1:E:181:VAL:CB	2:F:352:LYS:CE	2.61	0.71
1:E:256:GLN:HG2	2:R:407:TRP:CH2	2.25	0.71
1:K:210:TYR:CG	2:L:326:LYS:HD2	2.25	0.71
1:M:181:VAL:HA	2:N:352:LYS:NZ	2.04	0.71
1:M:210:TYR:CG	2:N:326:LYS:HD2	2.25	0.71
2:R:266:HIS:ND1	2:R:266:HIS:O	2.22	0.71
1:A:243:ARG:NH2	2:P:71:GLU:OE2	2.24	0.71
2:B:181:VAL:HG23	1:I:350:GLY:O	1.89	0.71
2:B:401:ARG:HG3	1:I:346:TRP:HB3	0.78	0.71
1:G:210:TYR:OH	2:H:325:MET:C	2.27	0.71
1:A:249:ASN:N	2:P:11:GLN:HE22	1.86	0.71
2:B:96:GLN:NE2	1:I:2:ARG:CG	2.29	0.71
1:K:179:THR:O	2:L:352:LYS:HB3	1.90	0.71
1:A:97:GLU:CD	2:B:2:ARG:NE	2.43	0.71
1:E:179:THR:O	2:F:352:LYS:HB3	1.90	0.71
2:F:97:SER:CB	1:K:133:GLN:HE22	2.03	0.71
1:K:176:GLN:HB3	2:L:333:LEU:CG	2.19	0.71
1:K:210:TYR:CD2	2:L:326:LYS:CG	2.72	0.71
1:A:101:ASN:H	2:B:254:LYS:HD2	1.53	0.71
1:A:210:TYR:CZ	2:B:326:LYS:CB	2.74	0.71
2:D:96:GLN:NE2	1:G:2:ARG:CG	2.29	0.71
2:F:266:HIS:ND1	2:F:266:HIS:O	2.22	0.71
1:G:97:GLU:CD	2:H:2:ARG:CZ	2.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:TYR:CD1	2:L:325:MET:SD	2.81	0.71
2:P:283:TYR:C	2:R:56:ALA:HB2	2.11	0.71
1:A:353:VAL:CB	2:P:179:ASP:OD1	2.31	0.71
2:F:404:PHE:CE2	1:K:258:ASN:C	2.63	0.71
1:G:11:GLN:OE1	2:H:247:GLN:O	2.09	0.71
1:G:210:TYR:CG	2:H:326:LYS:HG3	2.26	0.71
1:M:401:LYS:HD3	2:N:346:TRP:NE1	2.05	0.71
1:A:401:LYS:NZ	2:B:437:ASP:OD2	2.24	0.71
2:B:71:GLU:OE2	1:I:243:ARG:NH2	2.24	0.71
1:E:224:TYR:CE2	2:F:325:MET:HG3	2.25	0.71
1:K:96:LYS:NZ	2:L:130:ASP:OD2	2.22	0.71
1:K:97:GLU:CD	2:L:2:ARG:NE	2.44	0.71
1:Q:100:ALA:HB1	2:R:254:LYS:HA	1.70	0.71
1:C:401:LYS:CD	2:D:346:TRP:CG	2.74	0.71
1:M:176:GLN:HB3	2:N:333:LEU:CD1	2.21	0.71
1:A:394:LYS:HG2	2:B:348:PRO:CB	2.21	0.71
1:C:249:ASN:H	2:N:11:GLN:NE2	1.87	0.71
2:B:56:ALA:HB1	2:D:283:TYR:CA	2.19	0.70
1:G:97:GLU:CD	2:H:2:ARG:NE	2.44	0.70
1:I:181:VAL:HG23	2:J:352:LYS:HE2	1.72	0.70
1:M:176:GLN:OE1	2:N:333:LEU:CD1	2.35	0.70
1:M:401:LYS:HD3	2:N:346:TRP:CD1	2.24	0.70
1:A:348:PRO:HG3	2:P:398:MET:SD	2.32	0.70
1:C:329:ASN:OD1	2:N:177:VAL:HG21	1.86	0.70
1:E:249:ASN:H	2:R:11:GLN:NE2	1.88	0.70
1:Q:407:TRP:NE1	2:R:260:VAL:HB	2.05	0.70
2:F:177:VAL:HG21	1:K:329:ASN:OD1	1.90	0.70
1:G:177:VAL:CG1	2:H:329:ASP:HA	2.18	0.70
1:M:181:VAL:HA	2:N:352:LYS:HE3	0.70	0.70
1:A:97:GLU:CD	2:B:2:ARG:CZ	2.57	0.70
1:K:210:TYR:OH	2:L:325:MET:C	2.29	0.70
1:M:105:ARG:NH2	2:N:253:ARG:NE	2.38	0.70
1:M:397:LEU:HB3	2:N:346:TRP:C	2.11	0.70
1:O:404:PHE:CA	2:P:261:PRO:HA	2.21	0.70
1:A:258:ASN:O	2:P:404:PHE:CE2	2.44	0.70
1:C:401:LYS:CG	2:D:346:TRP:HB3	2.22	0.70
1:E:210:TYR:CZ	2:F:326:LYS:CB	2.74	0.70
1:E:401:LYS:CG	2:F:346:TRP:HB3	2.22	0.70
1:G:176:GLN:HG3	2:H:333:LEU:HD21	1.72	0.70
1:Q:404:PHE:CA	2:R:261:PRO:HA	2.21	0.70
1:G:101:ASN:HB2	2:H:254:LYS:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:177:VAL:HG21	2:R:329:ASP:CA	2.21	0.70
2:D:407:TRP:CH2	1:G:256:GLN:HG2	2.27	0.70
1:G:181:VAL:HG23	2:H:352:LYS:HE2	1.73	0.70
1:K:401:LYS:HD3	2:L:346:TRP:NE1	2.06	0.70
1:O:407:TRP:NE1	2:P:260:VAL:HB	2.05	0.70
1:A:329:ASN:CG	2:P:177:VAL:HG21	2.11	0.70
1:C:238:ILE:O	1:C:238:ILE:CG2	2.40	0.70
1:C:401:LYS:CD	2:D:346:TRP:CD1	2.75	0.70
1:M:100:ALA:HB1	2:N:254:LYS:HA	1.72	0.70
1:Q:105:ARG:CZ	2:R:253:ARG:HE	2.03	0.70
2:B:11:GLN:OE1	1:I:247:ALA:O	2.09	0.70
1:G:176:GLN:HB3	2:H:333:LEU:CG	2.22	0.70
1:G:238:ILE:O	1:G:238:ILE:CG2	2.40	0.70
1:C:2:ARG:HG3	2:N:96:GLN:HE22	0.55	0.69
1:M:401:LYS:CD	2:N:346:TRP:CG	2.75	0.69
2:P:283:TYR:CA	2:R:56:ALA:HB2	2.20	0.69
1:A:210:TYR:HB3	2:B:326:LYS:CE	2.21	0.69
1:E:101:ASN:H	2:F:254:LYS:HD2	1.55	0.69
1:I:394:LYS:HG2	2:J:348:PRO:CB	2.22	0.69
1:M:238:ILE:O	1:M:238:ILE:CG2	2.40	0.69
1:M:397:LEU:CB	2:N:346:TRP:O	2.39	0.69
1:O:404:PHE:CZ	2:P:314:THR:HG22	2.24	0.69
1:A:176:GLN:CG	2:B:333:LEU:HD21	2.22	0.69
2:B:283:TYR:HB3	2:F:62:VAL:CG2	2.21	0.69
1:E:394:LYS:NZ	2:F:349:ASN:ND2	2.41	0.69
1:O:179:THR:HG22	2:P:353:THR:CB	2.21	0.69
1:Q:238:ILE:O	1:Q:238:ILE:CG2	2.40	0.69
2:B:398:MET:HG3	1:I:348:PRO:HD3	1.74	0.69
2:D:11:GLN:OE1	1:G:247:ALA:O	2.10	0.69
1:E:404:PHE:HE2	2:F:258:ASN:O	1.72	0.69
1:I:404:PHE:CZ	2:J:314:THR:CG2	2.75	0.69
1:A:210:TYR:CB	2:B:326:LYS:HD2	2.21	0.69
1:C:179:THR:HG22	2:D:353:THR:HG1	1.57	0.69
1:C:348:PRO:HD3	2:N:398:MET:HG3	1.71	0.69
1:K:394:LYS:HG2	2:L:348:PRO:CB	2.23	0.69
1:A:179:THR:HB	2:B:353:THR:O	1.92	0.69
1:C:210:TYR:CZ	2:D:326:LYS:CB	2.75	0.69
1:K:238:ILE:O	1:K:238:ILE:CG2	2.40	0.69
1:M:401:LYS:CG	2:N:346:TRP:HB3	2.22	0.69
1:E:238:ILE:O	1:E:238:ILE:CG2	2.40	0.69
1:K:181:VAL:HB	2:L:352:LYS:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:404:PHE:CA	2:N:261:PRO:HA	2.22	0.69
1:Q:401:LYS:CD	2:R:346:TRP:CG	2.75	0.69
1:C:100:ALA:C	2:D:254:LYS:HD2	2.12	0.69
1:C:176:GLN:CG	2:D:333:LEU:HD21	2.23	0.69
1:C:181:VAL:CB	2:D:352:LYS:CE	2.64	0.69
1:C:243:ARG:NH2	2:N:71:GLU:OE2	2.25	0.69
2:D:71:GLU:OE2	1:G:243:ARG:NH2	2.25	0.69
1:E:260:VAL:HB	2:R:407:TRP:HZ2	1.57	0.69
1:O:283:HIS:HA	1:Q:56:THR:CG2	2.17	0.69
1:A:177:VAL:HG21	2:B:329:ASP:CA	2.23	0.69
1:C:210:TYR:CB	2:D:326:LYS:HD2	2.22	0.69
1:E:176:GLN:HB2	2:F:333:LEU:HD22	1.71	0.69
1:E:210:TYR:HB3	2:F:326:LYS:CE	2.22	0.69
2:B:176:LYS:HD3	1:I:333:ALA:HB2	1.74	0.69
2:B:282:GLN:O	2:F:60:LYS:HB2	1.92	0.69
1:E:348:PRO:CG	2:R:398:MET:SD	2.81	0.69
1:E:353:VAL:CB	2:R:179:ASP:OD1	2.36	0.69
2:F:176:LYS:HD3	1:K:333:ALA:HB2	1.74	0.69
1:K:179:THR:CG2	2:L:353:THR:HG1	2.03	0.69
1:O:176:GLN:HB3	2:P:333:LEU:CD1	2.22	0.69
2:B:407:TRP:CH2	1:I:256:GLN:HG2	2.27	0.68
1:C:181:VAL:HA	2:D:352:LYS:NZ	2.08	0.68
1:I:179:THR:O	2:J:352:LYS:HB3	1.93	0.68
1:Q:101:ASN:HD22	2:R:258:ASN:HD21	1.41	0.68
1:Q:401:LYS:HD3	2:R:346:TRP:CD1	2.25	0.68
2:B:177:VAL:CG2	1:I:329:ASN:CG	2.61	0.68
1:C:177:VAL:HG21	2:D:329:ASP:CA	2.23	0.68
1:C:394:LYS:HG2	2:D:348:PRO:CB	2.24	0.68
1:I:238:ILE:O	1:I:238:ILE:CG2	2.40	0.68
1:K:404:PHE:CZ	2:L:314:THR:CG2	2.75	0.68
1:O:394:LYS:HA	2:P:348:PRO:CG	2.19	0.68
2:B:404:PHE:CZ	1:I:258:ASN:O	2.46	0.68
1:C:249:ASN:N	2:N:11:GLN:HE22	1.90	0.68
1:C:329:ASN:CB	2:N:177:VAL:HG21	2.23	0.68
1:E:249:ASN:N	2:R:11:GLN:HE22	1.90	0.68
1:E:407:TRP:CZ2	2:F:256:ALA:O	2.47	0.68
1:I:179:THR:HB	2:J:353:THR:O	1.92	0.68
1:O:210:TYR:CG	2:P:326:LYS:CD	2.76	0.68
1:A:11:GLN:CD	2:B:247:GLN:O	2.31	0.68
1:A:283:HIS:HA	1:E:56:THR:CG2	2.17	0.68
1:E:179:THR:HA	2:F:353:THR:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:TRP:CZ2	2:F:260:VAL:HB	2.28	0.68
1:M:397:LEU:HD22	2:N:345:GLU:O	1.93	0.68
1:A:238:ILE:O	1:A:238:ILE:CG2	2.40	0.68
1:E:176:GLN:CG	2:F:333:LEU:HD21	2.24	0.68
1:O:407:TRP:CB	2:P:257:VAL:HG13	2.24	0.68
1:A:401:LYS:CG	2:B:346:TRP:HB3	2.23	0.68
2:F:11:GLN:OE1	1:K:247:ALA:O	2.10	0.68
1:I:401:LYS:HD3	2:J:346:TRP:NE1	2.07	0.68
2:P:283:TYR:HA	2:R:56:ALA:HB2	1.69	0.68
1:A:249:ASN:ND2	2:P:11:GLN:OE1	2.27	0.68
1:C:348:PRO:CG	2:N:398:MET:SD	2.82	0.68
1:E:258:ASN:O	2:R:404:PHE:CZ	2.45	0.68
1:O:238:ILE:O	1:O:238:ILE:CG2	2.40	0.68
1:O:401:LYS:HD3	2:P:346:TRP:CG	2.29	0.68
1:A:401:LYS:CD	2:B:346:TRP:CG	2.77	0.68
1:C:210:TYR:HB3	2:D:326:LYS:CE	2.23	0.68
1:E:401:LYS:HD3	2:F:346:TRP:NE1	2.08	0.68
1:Q:401:LYS:CG	2:R:346:TRP:HB3	2.23	0.68
1:A:401:LYS:CD	2:B:346:TRP:CD1	2.77	0.68
1:C:179:THR:HB	2:D:353:THR:O	1.94	0.68
1:C:176:GLN:HB2	2:D:333:LEU:HD22	1.72	0.67
1:M:407:TRP:HE1	2:N:260:VAL:HB	1.58	0.67
2:J:283:TYR:C	2:L:56:ALA:HB2	2.13	0.67
2:B:11:GLN:NE2	1:I:249:ASN:H	1.92	0.67
1:C:11:GLN:CD	2:D:247:GLN:O	2.33	0.67
1:G:179:THR:HB	2:H:353:THR:O	1.94	0.67
2:N:282:GLN:O	2:P:60:LYS:CB	2.41	0.67
1:A:407:TRP:CZ2	2:B:256:ALA:O	2.48	0.67
2:D:404:PHE:CZ	1:G:258:ASN:O	2.47	0.67
1:E:224:TYR:CD1	2:F:325:MET:SD	2.86	0.67
1:G:401:LYS:HD3	2:H:346:TRP:NE1	2.07	0.67
2:J:282:GLN:O	2:L:60:LYS:CB	2.41	0.67
1:K:177:VAL:HG21	2:L:329:ASP:CA	2.25	0.67
1:Q:397:LEU:HB3	2:R:346:TRP:C	2.14	0.67
1:G:179:THR:O	2:H:352:LYS:HB3	1.94	0.67
1:I:179:THR:CA	2:J:353:THR:H	2.08	0.67
1:M:181:VAL:HG23	2:N:352:LYS:HE2	1.76	0.67
1:Q:397:LEU:HD22	2:R:345:GLU:O	1.94	0.67
2:B:177:VAL:HG21	1:I:329:ASN:OD1	1.90	0.67
1:C:179:THR:O	2:D:352:LYS:HB3	1.94	0.67
1:I:210:TYR:CG	2:J:326:LYS:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:VAL:CB	2:N:352:LYS:CE	2.62	0.67
1:A:179:THR:HG21	2:B:248:LEU:HD13	1.76	0.67
1:A:181:VAL:HB	2:B:352:LYS:HG3	1.76	0.67
1:C:350:GLY:CA	2:N:181:VAL:HA	2.22	0.67
2:D:176:LYS:HD3	1:G:333:ALA:HB2	1.75	0.67
1:E:210:TYR:CZ	2:F:326:LYS:HB2	2.29	0.67
1:I:401:LYS:HD3	2:J:346:TRP:CD1	2.28	0.67
1:A:105:ARG:CZ	2:B:253:ARG:NE	2.57	0.67
1:E:101:ASN:HB2	2:F:254:LYS:CG	2.24	0.67
1:C:256:GLN:O	2:N:407:TRP:CZ2	2.48	0.67
1:Q:243:ARG:NE	1:Q:243:ARG:HA	2.10	0.67
1:E:100:ALA:C	2:F:254:LYS:HD2	2.14	0.67
1:E:401:LYS:CG	2:F:346:TRP:CD2	2.78	0.67
1:G:101:ASN:H	2:H:254:LYS:HD2	1.54	0.67
1:K:101:ASN:HB2	2:L:254:LYS:CG	2.24	0.67
1:K:181:VAL:HG23	2:L:352:LYS:HE2	1.77	0.67
1:O:177:VAL:HB	2:P:329:ASP:HB3	1.77	0.67
1:A:2:ARG:HG3	2:P:96:GLN:HE22	0.51	0.66
1:A:179:THR:O	2:B:352:LYS:HB3	1.93	0.66
2:B:11:GLN:OE1	1:I:249:ASN:ND2	2.28	0.66
1:C:243:ARG:NE	1:C:243:ARG:HA	2.10	0.66
1:E:105:ARG:NH2	2:F:253:ARG:NE	2.41	0.66
1:G:243:ARG:HA	1:G:243:ARG:NE	2.10	0.66
1:K:401:LYS:CD	2:L:346:TRP:CD2	2.78	0.66
1:O:179:THR:HG21	2:P:248:LEU:HD13	1.76	0.66
1:O:394:LYS:C	2:P:348:PRO:HG3	2.16	0.66
1:O:397:LEU:HB2	2:P:348:PRO:HD3	1.76	0.66
1:Q:407:TRP:HE1	2:R:260:VAL:HB	1.60	0.66
1:A:181:VAL:CB	2:B:352:LYS:CE	2.65	0.66
1:A:210:TYR:CZ	2:B:326:LYS:HB2	2.29	0.66
1:A:283:HIS:C	1:E:56:THR:CG2	2.63	0.66
1:E:101:ASN:CB	2:F:254:LYS:CE	2.42	0.66
1:E:243:ARG:HA	1:E:243:ARG:NE	2.10	0.66
1:E:401:LYS:CD	2:F:346:TRP:CD2	2.78	0.66
1:K:243:ARG:NE	1:K:243:ARG:HA	2.10	0.66
1:A:210:TYR:OH	2:B:325:MET:C	2.34	0.66
1:A:352:LYS:CA	2:P:179:ASP:O	2.41	0.66
1:C:97:GLU:CD	2:D:2:ARG:CZ	2.62	0.66
1:C:249:ASN:ND2	2:N:11:GLN:OE1	2.28	0.66
1:C:407:TRP:CZ2	2:D:256:ALA:O	2.49	0.66
2:D:179:ASP:OD1	1:G:353:VAL:CB	2.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:TYR:CD1	2:J:325:MET:SD	2.83	0.66
1:C:210:TYR:CZ	2:D:326:LYS:HB2	2.30	0.66
1:G:394:LYS:HG2	2:H:348:PRO:CB	2.26	0.66
1:O:407:TRP:HE1	2:P:260:VAL:HB	1.59	0.66
1:Q:397:LEU:CB	2:R:346:TRP:O	2.43	0.66
1:A:176:GLN:HB2	2:B:333:LEU:HD22	1.71	0.66
2:D:11:GLN:OE1	1:G:249:ASN:ND2	2.28	0.66
1:G:404:PHE:CZ	2:H:314:THR:CG2	2.78	0.66
1:I:243:ARG:NE	1:I:243:ARG:HA	2.10	0.66
1:K:100:ALA:HB1	2:L:254:LYS:HA	1.77	0.66
1:Q:176:GLN:OE1	2:R:333:LEU:CD1	2.38	0.66
1:A:348:PRO:HD2	2:P:398:MET:HG2	1.78	0.66
1:C:179:THR:HG21	2:D:248:LEU:HD13	1.77	0.66
1:E:11:GLN:OE1	2:F:247:GLN:O	2.14	0.66
1:E:394:LYS:HG2	2:F:348:PRO:CB	2.26	0.66
1:E:398:MET:HG3	2:F:348:PRO:HD2	1.77	0.66
1:A:243:ARG:NE	1:A:243:ARG:HA	2.10	0.66
1:E:404:PHE:CZ	2:F:314:THR:CG2	2.78	0.66
1:G:401:LYS:HD3	2:H:346:TRP:CD1	2.29	0.66
1:M:101:ASN:CA	2:N:254:LYS:CE	2.74	0.66
1:O:101:ASN:HD22	2:P:258:ASN:ND2	1.94	0.66
2:B:62:VAL:CG2	2:D:283:TYR:HB3	2.26	0.66
1:G:401:LYS:HD3	2:H:346:TRP:CG	2.29	0.66
1:I:105:ARG:CZ	2:J:253:ARG:NE	2.59	0.66
1:I:401:LYS:CD	2:J:346:TRP:CD2	2.79	0.66
1:O:243:ARG:HA	1:O:243:ARG:NE	2.10	0.66
1:M:179:THR:HG21	2:N:248:LEU:HD13	1.77	0.65
1:A:176:GLN:HG3	2:B:333:LEU:HD21	1.78	0.65
1:O:394:LYS:O	2:P:348:PRO:HG3	1.96	0.65
1:Q:179:THR:CG2	2:R:353:THR:HG1	2.08	0.65
1:C:333:ALA:HB2	2:N:176:LYS:HD3	1.78	0.65
1:G:401:LYS:CD	2:H:346:TRP:CD2	2.76	0.65
2:N:283:TYR:C	2:P:56:ALA:HB2	2.17	0.65
1:Q:177:VAL:CG1	2:R:329:ASP:HA	2.16	0.65
1:Q:210:TYR:HB3	2:R:326:LYS:HE2	1.77	0.65
1:M:101:ASN:HB2	2:N:254:LYS:HG3	1.78	0.65
1:M:243:ARG:HA	1:M:243:ARG:NE	2.10	0.65
1:O:176:GLN:HG3	2:P:333:LEU:CD2	2.22	0.65
2:B:282:GLN:O	2:F:60:LYS:CB	2.44	0.65
1:C:210:TYR:OH	2:D:325:MET:C	2.35	0.65
1:E:179:THR:HG22	2:F:353:THR:HG1	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:283:TYR:HD2	2:L:62:VAL:CG2	1.96	0.65
1:A:210:TYR:CG	2:B:326:LYS:CG	2.79	0.65
1:C:329:ASN:CG	2:N:177:VAL:HG21	2.16	0.65
1:E:329:ASN:CG	2:R:177:VAL:HG21	2.16	0.65
1:G:179:THR:HG21	2:H:248:LEU:HD13	1.78	0.65
1:I:401:LYS:HD3	2:J:346:TRP:CG	2.29	0.65
2:B:381:SER:OG	2:B:382:THR:N	2.29	0.65
1:C:181:VAL:HB	2:D:352:LYS:HG3	1.78	0.65
1:E:97:GLU:CD	2:F:2:ARG:CZ	2.62	0.65
1:E:210:TYR:CB	2:F:326:LYS:HD2	2.26	0.65
1:E:348:PRO:HG3	2:R:398:MET:SD	2.37	0.65
1:E:350:GLY:CA	2:R:181:VAL:HA	2.24	0.65
1:I:100:ALA:HB1	2:J:254:LYS:HA	1.78	0.65
1:M:210:TYR:CG	2:N:326:LYS:HB2	2.30	0.65
1:O:181:VAL:HG12	2:P:258:ASN:OD1	1.96	0.65
1:O:210:TYR:CE2	2:P:326:LYS:CB	2.77	0.65
1:O:210:TYR:CG	2:P:326:LYS:CB	2.80	0.65
2:P:381:SER:OG	2:P:382:THR:N	2.29	0.65
1:A:404:PHE:CZ	2:B:314:THR:CG2	2.78	0.65
1:I:179:THR:HG21	2:J:248:LEU:HD13	1.78	0.65
1:A:56:THR:CG2	1:C:283:HIS:HA	2.23	0.65
1:A:181:VAL:HA	2:B:352:LYS:NZ	2.09	0.65
1:A:333:ALA:HB2	2:P:176:LYS:HD3	1.78	0.65
1:C:97:GLU:CD	2:D:2:ARG:NE	2.49	0.65
2:D:11:GLN:NE2	1:G:249:ASN:H	1.93	0.65
2:F:407:TRP:CH2	1:K:256:GLN:HG2	2.32	0.65
2:J:381:SER:OG	2:J:382:THR:N	2.29	0.65
1:K:105:ARG:NH2	2:L:253:ARG:NE	2.45	0.65
1:O:406:HIS:HE1	2:P:260:VAL:HG12	1.54	0.65
2:B:11:GLN:HE22	1:I:249:ASN:N	1.95	0.65
2:B:407:TRP:HZ2	1:I:260:VAL:HB	1.61	0.65
2:D:177:VAL:HG21	1:G:329:ASN:OD1	1.90	0.65
2:D:398:MET:HG3	1:G:348:PRO:HD3	1.78	0.65
2:F:398:MET:HG3	1:K:348:PRO:HD3	1.79	0.65
1:G:224:TYR:CD1	2:H:325:MET:SD	2.86	0.65
1:G:401:LYS:CG	2:H:346:TRP:CD2	2.80	0.64
1:O:15:GLN:OE1	1:O:15:GLN:HA	1.98	0.64
1:A:15:GLN:OE1	1:A:15:GLN:HA	1.98	0.64
2:B:60:LYS:HB2	2:D:282:GLN:O	1.97	0.64
1:C:348:PRO:HG3	2:N:398:MET:SD	2.38	0.64
1:G:15:GLN:OE1	1:G:15:GLN:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:VAL:HG12	2:J:258:ASN:OD1	1.96	0.64
1:I:210:TYR:CG	2:J:326:LYS:CD	2.80	0.64
1:K:179:THR:HB	2:L:353:THR:O	1.97	0.64
1:M:11:GLN:HE22	2:N:247:GLN:C	1.99	0.64
1:O:73:THR:HG21	2:P:245:PRO:HA	1.79	0.64
1:A:11:GLN:OE1	2:B:247:GLN:O	2.16	0.64
1:C:15:GLN:OE1	1:C:15:GLN:HA	1.98	0.64
2:F:11:GLN:NE2	1:K:249:ASN:H	1.94	0.64
1:I:407:TRP:CE3	2:J:257:VAL:HG22	2.31	0.64
1:M:15:GLN:HA	1:M:15:GLN:OE1	1.98	0.64
1:I:15:GLN:OE1	1:I:15:GLN:HA	1.98	0.64
1:K:401:LYS:CG	2:L:346:TRP:CD2	2.80	0.64
1:O:101:ASN:HB2	2:P:254:LYS:HG3	1.79	0.64
3:O:501:GTP:O1A	2:P:249:ASN:HB3	1.96	0.64
1:Q:15:GLN:OE1	1:Q:15:GLN:HA	1.98	0.64
1:Q:101:ASN:CA	2:R:254:LYS:CE	2.75	0.64
1:C:352:LYS:CA	2:N:179:ASP:O	2.44	0.64
1:E:15:GLN:HA	1:E:15:GLN:OE1	1.98	0.64
2:F:11:GLN:OE1	1:K:249:ASN:ND2	2.30	0.64
2:F:181:VAL:HG23	1:K:350:GLY:O	1.95	0.64
1:G:407:TRP:CE3	2:H:257:VAL:HG22	2.31	0.64
1:Q:179:THR:HG22	2:R:353:THR:CB	2.26	0.64
1:A:176:GLN:CG	2:B:333:LEU:CD2	2.75	0.64
1:E:346:TRP:HB3	2:R:401:ARG:HG3	0.78	0.64
1:K:15:GLN:OE1	1:K:15:GLN:HA	1.98	0.64
1:K:105:ARG:CZ	2:L:253:ARG:NE	2.61	0.64
1:E:105:ARG:CZ	2:F:253:ARG:NE	2.61	0.64
1:M:179:THR:HG22	2:N:353:THR:CB	2.25	0.64
1:O:179:THR:HA	2:P:353:THR:N	2.10	0.64
2:D:177:VAL:CG2	1:G:329:ASN:CG	2.65	0.64
1:E:329:ASN:CB	2:R:177:VAL:HG21	2.28	0.64
1:E:333:ALA:HB2	2:R:176:LYS:HD3	1.79	0.64
1:G:181:VAL:HG12	2:H:258:ASN:OD1	1.97	0.64
1:I:101:ASN:CA	2:J:254:LYS:HE3	2.23	0.64
3:M:501:GTP:O1A	2:N:249:ASN:HB3	1.97	0.64
1:A:181:VAL:HG12	2:B:258:ASN:OD1	1.98	0.64
1:C:404:PHE:CZ	2:D:314:THR:CG2	2.79	0.64
1:O:283:HIS:C	1:Q:56:THR:CG2	2.66	0.64
1:Q:210:TYR:CB	2:R:326:LYS:CD	2.74	0.64
1:A:210:TYR:CG	2:B:326:LYS:HG3	2.33	0.64
1:C:105:ARG:CZ	2:D:253:ARG:NE	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:181:VAL:HA	2:P:352:LYS:HE3	0.64	0.64
2:D:181:VAL:HG23	1:G:350:GLY:O	1.94	0.63
1:G:100:ALA:HB1	2:H:254:LYS:HA	1.80	0.63
1:G:179:THR:CA	2:H:353:THR:H	2.11	0.63
1:K:179:THR:CA	2:L:353:THR:H	2.11	0.63
1:A:177:VAL:HG22	2:B:329:ASP:O	1.96	0.63
2:B:398:MET:SD	1:I:348:PRO:CG	2.86	0.63
1:C:258:ASN:O	2:N:404:PHE:CE2	2.50	0.63
1:O:210:TYR:HB3	2:P:326:LYS:HE2	1.79	0.63
1:C:179:THR:CG2	2:D:353:THR:HG1	2.11	0.63
1:E:100:ALA:HB1	2:F:254:LYS:HA	1.79	0.63
2:F:179:ASP:OD1	1:K:353:VAL:CB	2.41	0.63
2:J:283:TYR:CD2	2:L:62:VAL:CG2	2.74	0.63
1:Q:11:GLN:HE22	2:R:247:GLN:C	1.98	0.63
1:Q:181:VAL:HG23	2:R:352:LYS:HE2	1.79	0.63
1:C:176:GLN:CG	2:D:333:LEU:CD2	2.76	0.63
1:C:353:VAL:CB	2:N:179:ASP:OD1	2.35	0.63
1:K:176:GLN:HB3	2:L:333:LEU:CD1	2.28	0.63
1:O:181:VAL:HB	2:P:352:LYS:CG	2.28	0.63
1:A:105:ARG:NH2	2:B:253:ARG:NE	2.45	0.63
1:M:101:ASN:HD22	2:N:258:ASN:ND2	1.96	0.63
1:Q:210:TYR:CG	2:R:326:LYS:CD	2.81	0.63
1:C:210:TYR:CG	2:D:326:LYS:CG	2.81	0.63
1:E:177:VAL:HG22	2:F:329:ASP:O	1.98	0.63
1:G:210:TYR:CG	2:H:326:LYS:HB2	2.31	0.63
1:I:407:TRP:CB	2:J:257:VAL:HG13	2.28	0.63
2:N:283:TYR:CA	2:P:56:ALA:HB2	2.26	0.63
1:K:407:TRP:CE3	2:L:257:VAL:HG22	2.33	0.63
1:O:105:ARG:HH22	2:P:253:ARG:NH2	1.95	0.63
1:A:256:GLN:CG	2:P:407:TRP:CH2	2.82	0.63
1:C:105:ARG:NH2	2:D:253:ARG:NE	2.46	0.63
2:F:404:PHE:CZ	1:K:258:ASN:O	2.52	0.63
1:I:283:HIS:HA	1:K:56:THR:CG2	2.21	0.63
1:M:176:GLN:HG3	2:N:333:LEU:CD2	2.27	0.63
1:O:101:ASN:CB	2:P:254:LYS:CD	2.69	0.63
2:B:179:ASP:OD1	1:I:353:VAL:CB	2.38	0.62
1:I:105:ARG:NH2	2:J:253:ARG:NE	2.47	0.62
1:K:401:LYS:HD3	2:L:346:TRP:CD1	2.31	0.62
1:C:176:GLN:HG3	2:D:333:LEU:HD21	1.80	0.62
1:G:105:ARG:CZ	2:H:253:ARG:NE	2.63	0.62
1:G:407:TRP:CG	2:H:257:VAL:HG13	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:ARG:CZ	2:J:253:ARG:HE	2.11	0.62
1:A:407:TRP:NE1	2:B:260:VAL:HB	2.15	0.62
2:D:11:GLN:HE22	1:G:249:ASN:N	1.97	0.62
2:H:282:GLN:O	2:J:60:LYS:CB	2.46	0.62
2:H:283:TYR:CA	2:J:56:ALA:HB2	2.24	0.62
1:M:283:HIS:HA	1:O:56:THR:CG2	2.26	0.62
1:Q:73:THR:HG21	2:R:245:PRO:HA	1.82	0.62
1:K:407:TRP:CZ2	2:L:260:VAL:HB	2.34	0.62
1:M:181:VAL:HG12	2:N:258:ASN:OD1	2.00	0.62
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.48	0.62
1:C:398:MET:HG3	2:D:348:PRO:HD2	1.81	0.62
1:E:249:ASN:ND2	2:R:11:GLN:OE1	2.32	0.62
1:G:283:HIS:HA	1:I:56:THR:CG2	2.26	0.62
1:I:404:PHE:CZ	2:J:314:THR:HG21	2.34	0.62
2:N:381:SER:OG	2:N:382:THR:N	2.29	0.62
1:O:100:ALA:C	2:P:254:LYS:CD	2.66	0.62
1:C:11:GLN:OE1	2:D:247:GLN:O	2.18	0.62
1:E:256:GLN:O	2:R:407:TRP:CZ2	2.53	0.62
2:F:11:GLN:HE22	1:K:249:ASN:N	1.97	0.62
1:I:394:LYS:HZ3	2:J:349:ASN:ND2	1.95	0.62
1:Q:101:ASN:HB2	2:R:254:LYS:HG3	1.80	0.62
1:C:401:LYS:HD3	2:D:346:TRP:NE1	2.14	0.62
1:E:407:TRP:NE1	2:F:260:VAL:HB	2.15	0.62
1:G:177:VAL:HG11	2:H:329:ASP:OD1	1.99	0.62
1:I:101:ASN:HD22	2:J:258:ASN:HD21	1.48	0.62
1:I:283:HIS:HB3	1:K:62:VAL:HG22	1.81	0.62
1:K:177:VAL:CG1	2:L:329:ASP:HA	2.20	0.62
1:E:210:TYR:CG	2:F:326:LYS:CG	2.82	0.62
1:M:406:HIS:HE1	2:N:260:VAL:HG12	1.57	0.62
1:A:179:THR:CA	2:B:353:THR:H	2.13	0.62
1:A:283:HIS:C	1:E:56:THR:HG21	2.18	0.62
2:D:381:SER:OG	2:D:382:THR:N	2.29	0.62
1:E:352:LYS:CA	2:R:179:ASP:O	2.46	0.62
2:H:283:TYR:C	2:J:56:ALA:HB2	2.19	0.62
1:I:210:TYR:CE2	2:J:326:LYS:CB	2.82	0.62
1:Q:101:ASN:HD22	2:R:258:ASN:ND2	1.98	0.62
1:A:105:ARG:CZ	2:B:253:ARG:HE	2.13	0.61
2:B:60:LYS:CB	2:D:282:GLN:O	2.48	0.61
1:E:177:VAL:HG21	2:F:329:ASP:CA	2.30	0.61
1:I:176:GLN:HB3	2:J:333:LEU:CD1	2.30	0.61
1:I:397:LEU:HD22	2:J:345:GLU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:CG	2:P:400:ARG:HH22	2.02	0.61
1:A:404:PHE:CZ	2:B:314:THR:HG21	2.36	0.61
1:A:435:VAL:HG22	2:P:401:ARG:NH2	2.14	0.61
1:C:177:VAL:HG22	2:D:329:ASP:O	1.96	0.61
1:C:210:TYR:CG	2:D:326:LYS:HG3	2.36	0.61
1:I:177:VAL:HB	2:J:329:ASP:HB3	1.81	0.61
1:K:105:ARG:CZ	2:L:253:ARG:HE	2.12	0.61
1:O:72:PRO:HB2	2:P:48:ARG:NH1	2.15	0.61
1:A:181:VAL:HG23	2:B:352:LYS:HE2	1.81	0.61
2:B:177:VAL:HG21	1:I:329:ASN:CB	2.31	0.61
1:G:177:VAL:HG11	2:H:329:ASP:CB	2.31	0.61
2:H:381:SER:OG	2:H:382:THR:N	2.29	0.61
1:I:407:TRP:CG	2:J:257:VAL:HG13	2.34	0.61
1:K:101:ASN:CA	2:L:254:LYS:HE3	2.24	0.61
1:K:394:LYS:HZ3	2:L:349:ASN:ND2	1.96	0.61
1:M:210:TYR:CG	2:N:326:LYS:CD	2.82	0.61
1:M:407:TRP:CB	2:N:257:VAL:HG13	2.30	0.61
1:C:181:VAL:HG12	2:D:258:ASN:OD1	2.00	0.61
1:K:210:TYR:CG	2:L:326:LYS:CD	2.84	0.61
1:M:179:THR:HA	2:N:353:THR:N	2.14	0.61
1:O:11:GLN:HE22	2:P:247:GLN:C	2.00	0.61
1:A:210:TYR:CD1	2:B:326:LYS:CB	2.75	0.61
1:C:177:VAL:HG11	2:D:329:ASP:OD1	2.00	0.61
1:C:181:VAL:HG23	2:D:352:LYS:HE2	1.82	0.61
1:E:181:VAL:HB	2:F:352:LYS:HG3	1.83	0.61
1:E:210:TYR:CG	2:F:326:LYS:HG3	2.35	0.61
1:I:101:ASN:CA	2:J:254:LYS:CE	2.78	0.61
1:O:100:ALA:HB1	2:P:254:LYS:CA	2.29	0.61
2:R:381:SER:OG	2:R:382:THR:N	2.29	0.61
1:E:176:GLN:HG3	2:F:333:LEU:HD21	1.83	0.61
1:I:176:GLN:OE1	2:J:333:LEU:CD1	2.42	0.61
1:M:394:LYS:HA	2:N:348:PRO:CG	2.24	0.61
1:C:101:ASN:H	2:D:254:LYS:HD2	1.56	0.61
1:C:407:TRP:NE1	2:D:260:VAL:HB	2.16	0.61
1:E:97:GLU:CD	2:F:2:ARG:NE	2.53	0.61
1:M:210:TYR:CG	2:N:326:LYS:CB	2.84	0.61
1:A:256:GLN:O	2:P:407:TRP:CE2	2.54	0.61
2:B:210:TYR:OH	1:I:325:PRO:HB2	2.01	0.61
1:I:283:HIS:C	1:K:56:THR:CG2	2.69	0.61
1:A:177:VAL:HG11	2:B:329:ASP:OD1	2.01	0.61
2:F:381:SER:OG	2:F:382:THR:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:TRP:CB	2:H:257:VAL:HG13	2.30	0.61
1:M:401:LYS:HD3	2:N:346:TRP:CG	2.35	0.61
2:D:210:TYR:OH	1:G:325:PRO:HB2	2.01	0.61
1:G:210:TYR:CG	2:H:326:LYS:CD	2.84	0.61
1:I:179:THR:CG2	2:J:353:THR:HG1	2.12	0.61
1:Q:407:TRP:CE2	2:R:260:VAL:HB	2.35	0.61
1:E:176:GLN:CG	2:F:333:LEU:CD2	2.79	0.60
2:F:210:TYR:OH	1:K:325:PRO:HB2	2.01	0.60
1:I:401:LYS:CG	2:J:346:TRP:CD2	2.84	0.60
1:K:401:LYS:HD3	2:L:346:TRP:CG	2.34	0.60
1:M:73:THR:HG21	2:N:245:PRO:HA	1.83	0.60
1:O:100:ALA:CA	2:P:254:LYS:CB	2.70	0.60
1:Q:181:VAL:N	2:R:352:LYS:CE	2.50	0.60
1:E:181:VAL:HG23	2:F:352:LYS:HE2	1.84	0.60
2:F:177:VAL:CG2	1:K:329:ASN:CG	2.68	0.60
1:G:105:ARG:NH2	2:H:253:ARG:NE	2.48	0.60
1:I:394:LYS:O	2:J:348:PRO:HG3	2.01	0.60
1:M:210:TYR:HB3	2:N:326:LYS:HE2	1.81	0.60
1:A:101:ASN:HB2	2:B:254:LYS:HG3	1.82	0.60
1:A:398:MET:HG3	2:B:348:PRO:HD2	1.82	0.60
1:A:407:TRP:HE1	2:B:260:VAL:HB	1.66	0.60
2:B:398:MET:SD	1:I:348:PRO:HG3	2.41	0.60
1:E:179:THR:CG2	2:F:353:THR:HG1	2.11	0.60
2:L:381:SER:OG	2:L:382:THR:N	2.29	0.60
1:Q:394:LYS:C	2:R:348:PRO:HG3	2.22	0.60
2:D:407:TRP:HZ2	1:G:260:VAL:HB	1.65	0.60
1:E:105:ARG:CZ	2:F:253:ARG:HE	2.14	0.60
1:E:407:TRP:CE2	2:F:260:VAL:HB	2.37	0.60
2:F:407:TRP:HZ2	1:K:260:VAL:HB	1.62	0.60
2:H:221:THR:N	2:H:222:PRO:HD3	2.17	0.60
1:M:397:LEU:HB2	2:N:348:PRO:HD3	1.83	0.60
1:O:97:GLU:OE2	2:P:2:ARG:N	2.35	0.60
1:Q:407:TRP:CZ2	2:R:260:VAL:HB	2.37	0.60
1:Q:407:TRP:CB	2:R:257:VAL:HG13	2.32	0.60
1:A:56:THR:CG2	1:C:283:HIS:C	2.69	0.60
2:D:221:THR:N	2:D:222:PRO:HD3	2.17	0.60
1:E:210:TYR:OH	2:F:325:MET:C	2.38	0.60
1:I:177:VAL:HG11	2:J:329:ASP:OD1	2.01	0.60
1:A:176:GLN:HB3	2:B:333:LEU:CG	2.30	0.60
1:C:348:PRO:HD2	2:N:398:MET:HG2	1.84	0.60
1:O:283:HIS:C	1:Q:56:THR:HG21	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:407:TRP:CG	2:P:257:VAL:HA	2.36	0.60
1:C:345:ASP:CG	2:N:400:ARG:HH22	2.04	0.60
2:F:221:THR:N	2:F:222:PRO:HD3	2.16	0.60
1:G:394:LYS:O	2:H:348:PRO:HG3	2.02	0.60
2:L:221:THR:N	2:L:222:PRO:HD3	2.17	0.60
2:N:221:THR:N	2:N:222:PRO:HD3	2.17	0.60
1:O:181:VAL:N	2:P:352:LYS:CE	2.52	0.60
1:O:403:ALA:HB1	2:P:261:PRO:HB3	1.83	0.60
1:A:100:ALA:HB1	2:B:254:LYS:HA	1.82	0.60
1:A:210:TYR:CD2	2:B:326:LYS:CG	2.84	0.60
3:A:501:GTP:O1A	2:B:249:ASN:HB3	2.02	0.60
1:C:256:GLN:CG	2:N:407:TRP:CH2	2.85	0.60
1:G:101:ASN:CA	2:H:254:LYS:HE3	2.26	0.60
1:I:283:HIS:HB3	1:K:62:VAL:CG2	2.32	0.60
1:K:100:ALA:HA	2:L:254:LYS:HD2	1.84	0.60
1:K:404:PHE:CZ	2:L:314:THR:HG21	2.37	0.60
1:K:407:TRP:CB	2:L:257:VAL:HG13	2.32	0.60
1:A:401:LYS:HD3	2:B:346:TRP:NE1	2.17	0.60
1:E:179:THR:HB	2:F:353:THR:O	2.01	0.60
1:G:105:ARG:CZ	2:H:253:ARG:HE	2.14	0.60
1:Q:210:TYR:OH	2:R:326:LYS:HA	2.01	0.60
1:A:283:HIS:HB3	1:E:62:VAL:HG22	1.83	0.60
1:A:283:HIS:HB3	1:E:62:VAL:CG2	2.32	0.60
1:G:394:LYS:HZ3	2:H:349:ASN:ND2	1.98	0.60
1:Q:397:LEU:HD13	2:R:345:GLU:O	2.02	0.60
1:A:56:THR:HG21	1:C:283:HIS:C	2.22	0.59
2:B:179:ASP:O	1:I:352:LYS:CA	2.47	0.59
1:C:100:ALA:HB1	2:D:254:LYS:HA	1.82	0.59
1:C:176:GLN:HB3	2:D:333:LEU:CG	2.32	0.59
1:I:100:ALA:CA	2:J:254:LYS:HD2	2.32	0.59
1:K:407:TRP:CG	2:L:257:VAL:HG13	2.37	0.59
1:Q:394:LYS:O	2:R:348:PRO:HG3	2.01	0.59
2:R:221:THR:N	2:R:222:PRO:HD3	2.17	0.59
1:K:100:ALA:CA	2:L:254:LYS:HD2	2.32	0.59
1:M:404:PHE:CZ	2:N:314:THR:HG22	2.29	0.59
1:A:176:GLN:HB3	2:B:333:LEU:CD1	2.32	0.59
1:E:404:PHE:CA	2:F:261:PRO:HA	2.31	0.59
1:G:210:TYR:CE2	2:H:326:LYS:CB	2.84	0.59
1:K:179:THR:HG21	2:L:248:LEU:HD13	1.84	0.59
1:M:177:VAL:HB	2:N:329:ASP:HB3	1.84	0.59
1:O:100:ALA:CA	2:P:254:LYS:HD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:221:THR:N	2:P:222:PRO:HD3	2.17	0.59
1:Q:179:THR:HG21	2:R:248:LEU:HD13	1.83	0.59
1:A:258:ASN:CA	2:P:404:PHE:HE2	2.16	0.59
2:B:181:VAL:HA	1:I:350:GLY:CA	2.29	0.59
2:B:221:THR:N	2:B:222:PRO:HD3	2.17	0.59
1:G:177:VAL:HB	2:H:329:ASP:HB3	1.83	0.59
1:I:177:VAL:HG11	2:J:329:ASP:CB	2.31	0.59
1:K:210:TYR:HB3	2:L:326:LYS:HE2	1.83	0.59
1:M:394:LYS:C	2:N:348:PRO:HG3	2.22	0.59
1:O:404:PHE:HE2	2:P:258:ASN:C	2.05	0.59
1:O:407:TRP:CD1	2:P:257:VAL:O	2.55	0.59
1:C:101:ASN:HB2	2:D:254:LYS:HG3	1.84	0.59
1:C:105:ARG:CZ	2:D:253:ARG:HE	2.15	0.59
1:C:179:THR:CA	2:D:353:THR:H	2.15	0.59
1:K:181:VAL:HG12	2:L:258:ASN:OD1	2.02	0.59
1:M:407:TRP:CE2	2:N:260:VAL:HB	2.38	0.59
1:O:404:PHE:CE2	2:P:258:ASN:C	2.75	0.59
3:Q:501:GTP:O1A	2:R:249:ASN:HB3	2.01	0.59
1:A:258:ASN:O	2:P:404:PHE:HZ	1.84	0.59
1:A:346:TRP:HB3	2:P:401:ARG:HG3	0.67	0.59
1:E:179:THR:HG21	2:F:248:LEU:HD13	1.85	0.59
1:E:181:VAL:N	2:F:352:LYS:CE	2.54	0.59
1:G:176:GLN:OE1	2:H:333:LEU:CD1	2.44	0.59
2:J:221:THR:N	2:J:222:PRO:HD3	2.17	0.59
1:K:394:LYS:O	2:L:348:PRO:HG3	2.03	0.59
1:O:397:LEU:C	2:P:346:TRP:O	2.40	0.59
1:C:11:GLN:HG2	1:C:74:VAL:HG21	1.84	0.59
1:C:224:TYR:CD1	2:D:325:MET:SD	2.90	0.59
1:E:243:ARG:HH22	2:R:71:GLU:CD	2.06	0.59
1:M:11:GLN:HG2	1:M:74:VAL:HG21	1.84	0.59
1:G:176:GLN:HB3	2:H:333:LEU:CD1	2.33	0.59
1:I:210:TYR:CG	2:J:326:LYS:CB	2.86	0.59
1:K:11:GLN:HG2	1:K:74:VAL:HG21	1.84	0.59
1:E:11:GLN:HG2	1:E:74:VAL:HG21	1.84	0.59
1:O:100:ALA:CB	2:P:254:LYS:HB2	2.33	0.59
1:O:407:TRP:CE3	2:P:257:VAL:HG22	2.38	0.59
1:Q:11:GLN:HG2	1:Q:74:VAL:HG21	1.84	0.59
1:Q:210:TYR:CG	2:R:326:LYS:CB	2.86	0.59
1:Q:401:LYS:HD3	2:R:346:TRP:CG	2.37	0.59
1:A:258:ASN:HA	2:P:404:PHE:CE2	2.37	0.59
1:C:407:TRP:CZ2	2:D:260:VAL:HB	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:GLN:HG2	1:G:74:VAL:HG21	1.84	0.59
1:I:177:VAL:CB	2:J:329:ASP:HB3	2.33	0.59
1:K:177:VAL:HG11	2:L:329:ASP:CB	2.33	0.59
1:Q:176:GLN:HB3	2:R:333:LEU:HD13	1.84	0.59
1:A:345:ASP:OD1	2:P:400:ARG:NH2	2.34	0.58
1:E:394:LYS:HZ3	2:F:349:ASN:ND2	1.99	0.58
1:G:177:VAL:CB	2:H:329:ASP:HB3	2.33	0.58
1:M:394:LYS:O	2:N:348:PRO:HG3	2.02	0.58
1:O:101:ASN:CB	2:P:254:LYS:HG3	2.33	0.58
1:O:177:VAL:HG11	2:P:329:ASP:OD1	2.01	0.58
1:C:401:LYS:HD3	2:D:346:TRP:CD1	2.37	0.58
1:E:345:ASP:CG	2:R:400:ARG:HH22	2.05	0.58
1:I:11:GLN:HG2	1:I:74:VAL:HG21	1.84	0.58
1:M:97:GLU:OE2	2:N:2:ARG:N	2.35	0.58
1:O:177:VAL:CB	2:P:329:ASP:HB3	2.32	0.58
1:A:11:GLN:HG2	1:A:74:VAL:HG21	1.84	0.58
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.51	0.58
1:E:176:GLN:HB3	2:F:333:LEU:CG	2.31	0.58
2:F:179:ASP:O	1:K:352:LYS:CA	2.49	0.58
1:G:101:ASN:HD22	2:H:258:ASN:HD21	1.51	0.58
1:G:397:LEU:HD22	2:H:345:GLU:O	2.03	0.58
1:I:73:THR:HG21	2:J:245:PRO:HA	1.85	0.58
1:I:181:VAL:N	2:J:352:LYS:CE	2.55	0.58
1:K:404:PHE:CA	2:L:261:PRO:HA	2.33	0.58
1:M:101:ASN:CB	2:N:254:LYS:CD	2.74	0.58
1:O:11:GLN:HG2	1:O:74:VAL:HG21	1.84	0.58
1:A:97:GLU:OE2	2:B:2:ARG:N	2.36	0.58
2:D:179:ASP:O	1:G:352:LYS:CA	2.48	0.58
1:K:181:VAL:N	2:L:352:LYS:CE	2.51	0.58
1:M:210:TYR:CE1	2:N:326:LYS:CA	2.78	0.58
1:Q:394:LYS:HZ3	2:R:349:ASN:ND2	2.00	0.58
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.03	0.58
1:K:73:THR:HG21	2:L:245:PRO:HA	1.86	0.58
1:M:72:PRO:HB2	2:N:48:ARG:NH1	2.19	0.58
1:M:176:GLN:HB3	2:N:333:LEU:HD13	1.85	0.58
1:M:283:HIS:HB3	1:O:62:VAL:HG22	1.85	0.58
1:O:290:GLU:OE1	1:O:290:GLU:HA	2.04	0.58
1:O:407:TRP:CE2	2:P:260:VAL:HB	2.39	0.58
1:A:210:TYR:CG	2:B:326:LYS:HD2	2.38	0.58
1:A:224:TYR:CD1	2:B:325:MET:SD	2.88	0.58
1:A:401:LYS:HD3	2:B:346:TRP:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:CD1	2:D:326:LYS:CB	2.77	0.58
1:C:404:PHE:CZ	2:D:314:THR:HG21	2.38	0.58
1:E:176:GLN:HB3	2:F:333:LEU:CD1	2.34	0.58
1:K:407:TRP:NE1	2:L:260:VAL:HB	2.18	0.58
1:E:258:ASN:O	2:R:404:PHE:CE2	2.55	0.58
1:G:407:TRP:CZ2	2:H:260:VAL:HB	2.38	0.58
1:I:290:GLU:OE1	1:I:290:GLU:HA	2.04	0.58
1:I:407:TRP:NE1	2:J:260:VAL:HB	2.19	0.58
1:O:394:LYS:CG	2:P:348:PRO:HB2	2.26	0.58
2:B:177:VAL:HG21	1:I:329:ASN:CG	2.23	0.58
1:O:210:TYR:CB	2:P:326:LYS:CD	2.68	0.58
1:C:401:LYS:CG	2:D:346:TRP:CD2	2.87	0.58
1:C:404:PHE:CA	2:D:261:PRO:HA	2.34	0.58
1:K:176:GLN:O	2:L:333:LEU:HD13	2.04	0.58
2:N:283:TYR:HA	2:P:56:ALA:HB2	1.74	0.58
1:G:404:PHE:CZ	2:H:314:THR:HG21	2.38	0.58
1:K:290:GLU:OE1	1:K:290:GLU:HA	2.03	0.58
1:C:258:ASN:CA	2:N:404:PHE:HE2	2.18	0.57
1:C:407:TRP:HE1	2:D:260:VAL:HB	1.68	0.57
3:C:501:GTP:O1A	2:D:249:ASN:HB3	2.04	0.57
1:G:100:ALA:HA	2:H:254:LYS:HD2	1.86	0.57
1:G:100:ALA:CA	2:H:254:LYS:HD2	2.34	0.57
1:K:397:LEU:HD22	2:L:345:GLU:O	2.04	0.57
1:Q:290:GLU:HA	1:Q:290:GLU:OE1	2.03	0.57
1:A:404:PHE:CA	2:B:261:PRO:HA	2.34	0.57
1:E:290:GLU:OE1	1:E:290:GLU:HA	2.04	0.57
1:K:101:ASN:CA	2:L:254:LYS:CE	2.82	0.57
1:M:404:PHE:H	2:N:261:PRO:C	2.07	0.57
1:O:406:HIS:HE1	2:P:260:VAL:C	2.04	0.57
1:A:260:VAL:HB	2:P:407:TRP:HZ2	1.62	0.57
2:B:283:TYR:C	2:F:56:ALA:HB2	2.23	0.57
1:C:176:GLN:HB3	2:D:333:LEU:CD1	2.34	0.57
1:C:258:ASN:HA	2:N:404:PHE:CE2	2.38	0.57
1:G:283:HIS:C	1:I:56:THR:CG2	2.72	0.57
1:I:11:GLN:HE22	2:J:247:GLN:C	2.05	0.57
1:I:404:PHE:CA	2:J:261:PRO:HA	2.35	0.57
1:K:401:LYS:HG2	2:L:346:TRP:CD2	2.40	0.57
1:M:181:VAL:N	2:N:352:LYS:CE	2.54	0.57
1:M:290:GLU:OE1	1:M:290:GLU:HA	2.03	0.57
2:N:306:ASP:C	2:N:306:ASP:OD1	2.40	0.57
1:E:210:TYR:CG	2:F:326:LYS:HD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:LYS:HG2	2:F:346:TRP:CD2	2.40	0.57
1:G:101:ASN:CA	2:H:254:LYS:CE	2.81	0.57
1:M:177:VAL:HG11	2:N:329:ASP:OD1	2.05	0.57
1:O:177:VAL:HG11	2:P:329:ASP:CB	2.33	0.57
1:Q:176:GLN:O	2:R:333:LEU:HD13	2.03	0.57
1:C:401:LYS:HD3	2:D:346:TRP:CG	2.38	0.57
2:F:398:MET:SD	1:K:348:PRO:CG	2.93	0.57
1:G:283:HIS:C	1:I:56:THR:HG21	2.25	0.57
1:K:11:GLN:HE22	2:L:247:GLN:C	2.04	0.57
1:M:406:HIS:CE1	2:N:260:VAL:CG1	2.69	0.57
1:O:283:HIS:HB3	1:Q:62:VAL:CG2	2.35	0.57
1:A:62:VAL:HG22	1:C:283:HIS:HB3	1.86	0.57
1:C:290:GLU:OE1	1:C:290:GLU:HA	2.03	0.57
2:D:306:ASP:C	2:D:306:ASP:OD1	2.39	0.57
2:D:398:MET:SD	1:G:348:PRO:CG	2.92	0.57
1:E:404:PHE:CZ	2:F:314:THR:HG21	2.40	0.57
1:G:210:TYR:CG	2:H:326:LYS:CB	2.88	0.57
1:I:100:ALA:HA	2:J:254:LYS:HD2	1.86	0.57
1:M:100:ALA:HB1	2:N:254:LYS:CA	2.34	0.57
1:M:210:TYR:CE2	2:N:326:LYS:CB	2.84	0.57
1:O:179:THR:HG21	2:P:248:LEU:CD1	2.34	0.57
1:O:394:LYS:CA	2:P:348:PRO:CG	2.74	0.57
1:A:326:LYS:CB	2:P:210:TYR:CE2	2.85	0.57
2:B:400:ARG:HH22	1:I:345:ASP:CG	2.07	0.57
1:C:401:LYS:CD	2:D:346:TRP:CD2	2.84	0.57
1:I:397:LEU:HB2	2:J:348:PRO:HD3	1.87	0.57
1:K:101:ASN:HD22	2:L:258:ASN:HD21	1.53	0.57
1:Q:101:ASN:ND2	2:R:258:ASN:OD1	2.38	0.57
1:Q:177:VAL:HB	2:R:329:ASP:HB3	1.87	0.57
1:A:243:ARG:HH22	2:P:71:GLU:CD	2.08	0.57
1:C:210:TYR:CG	2:D:326:LYS:HD2	2.39	0.57
1:E:179:THR:CA	2:F:353:THR:H	2.18	0.57
1:G:290:GLU:OE1	1:G:290:GLU:HA	2.03	0.57
1:O:401:LYS:HG2	2:P:346:TRP:CG	2.37	0.57
1:Q:404:PHE:H	2:R:261:PRO:C	2.07	0.57
1:A:348:PRO:CG	2:P:398:MET:CG	2.82	0.57
1:C:346:TRP:HB3	2:N:401:ARG:HG3	0.70	0.57
1:M:100:ALA:C	2:N:254:LYS:CD	2.72	0.57
1:M:101:ASN:CB	2:N:254:LYS:HG3	2.35	0.57
1:O:181:VAL:HG11	2:P:258:ASN:O	2.04	0.57
1:O:283:HIS:HB3	1:Q:62:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:404:PHE:H	2:P:261:PRO:C	2.09	0.57
1:O:406:HIS:NE2	2:P:260:VAL:HG11	2.18	0.57
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.86	0.56
1:C:435:VAL:HG22	2:N:401:ARG:NH2	2.19	0.56
2:D:177:VAL:HG21	1:G:329:ASN:CB	2.35	0.56
1:E:262:TYR:HB3	1:E:263:PRO:HD2	1.86	0.56
1:E:435:VAL:HG22	2:R:401:ARG:NH2	2.19	0.56
1:G:11:GLN:HE22	2:H:247:GLN:C	2.07	0.56
1:K:210:TYR:OH	2:L:326:LYS:HA	2.03	0.56
1:O:262:TYR:HB3	1:O:263:PRO:HD2	1.86	0.56
1:Q:210:TYR:CG	2:R:326:LYS:HB2	2.33	0.56
1:A:346:TRP:HZ3	2:P:403:ALA:CB	1.79	0.56
1:G:283:HIS:HB3	1:I:62:VAL:HG22	1.87	0.56
1:M:100:ALA:CA	2:N:254:LYS:CB	2.73	0.56
1:O:394:LYS:HZ3	2:P:349:ASN:ND2	2.00	0.56
1:Q:100:ALA:CA	2:R:254:LYS:HD2	2.36	0.56
1:C:325:PRO:HB2	2:N:210:TYR:OH	2.05	0.56
1:E:210:TYR:CD2	2:F:326:LYS:CG	2.87	0.56
1:G:181:VAL:HB	2:H:352:LYS:CE	2.35	0.56
2:H:306:ASP:C	2:H:306:ASP:OD1	2.40	0.56
1:I:262:TYR:HB3	1:I:263:PRO:HD2	1.86	0.56
1:I:283:HIS:C	1:K:56:THR:HG21	2.24	0.56
1:I:407:TRP:CZ2	2:J:260:VAL:HB	2.40	0.56
1:M:181:VAL:HB	2:N:352:LYS:CG	2.35	0.56
1:M:397:LEU:HD13	2:N:345:GLU:O	2.05	0.56
1:O:100:ALA:C	2:P:254:LYS:CG	2.73	0.56
1:Q:179:THR:HA	2:R:353:THR:N	2.16	0.56
1:Q:262:TYR:HB3	1:Q:263:PRO:HD2	1.86	0.56
1:C:256:GLN:HG2	2:N:407:TRP:CZ2	2.41	0.56
1:E:326:LYS:CB	2:R:210:TYR:CE2	2.88	0.56
1:E:401:LYS:HD3	2:F:346:TRP:CD1	2.36	0.56
2:F:71:GLU:CD	1:K:243:ARG:HH22	2.09	0.56
1:Q:100:ALA:HB1	2:R:254:LYS:CA	2.34	0.56
1:Q:210:TYR:CE2	2:R:326:LYS:CB	2.86	0.56
1:C:97:GLU:OE2	2:D:2:ARG:N	2.39	0.56
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.86	0.56
1:E:11:GLN:HE22	2:F:247:GLN:C	2.07	0.56
1:E:401:LYS:HZ3	2:F:346:TRP:HE1	1.54	0.56
1:G:262:TYR:HB3	1:G:263:PRO:HD2	1.86	0.56
3:I:501:GTP:O1A	2:J:249:ASN:HB3	2.05	0.56
1:K:210:TYR:CE2	2:L:326:LYS:CB	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:TYR:HB3	1:K:263:PRO:HD2	1.86	0.56
1:M:262:TYR:HB3	1:M:263:PRO:HD2	1.86	0.56
1:A:329:ASN:CG	2:P:177:VAL:HG23	2.04	0.56
2:B:71:GLU:CD	1:I:243:ARG:HH22	2.09	0.56
1:E:101:ASN:HB2	2:F:254:LYS:HG3	1.88	0.56
1:I:283:HIS:O	1:K:62:VAL:HG21	2.05	0.56
1:Q:181:VAL:HG12	2:R:258:ASN:OD1	2.04	0.56
1:Q:401:LYS:CG	2:R:346:TRP:CD2	2.88	0.56
1:A:11:GLN:HE22	2:B:247:GLN:C	2.08	0.56
1:A:101:ASN:CA	2:B:254:LYS:HE3	2.31	0.56
1:Q:394:LYS:HA	2:R:348:PRO:CG	2.27	0.56
1:C:258:ASN:O	2:N:404:PHE:HZ	1.85	0.56
1:E:401:LYS:HD3	2:F:346:TRP:CG	2.38	0.56
1:G:404:PHE:CA	2:H:261:PRO:HA	2.36	0.56
1:I:210:TYR:HB3	2:J:326:LYS:HE2	1.84	0.56
1:M:407:TRP:CZ2	2:N:260:VAL:HB	2.41	0.56
1:O:210:TYR:CD2	2:P:326:LYS:CB	2.89	0.56
1:O:407:TRP:CG	2:P:257:VAL:HG13	2.40	0.56
1:A:401:LYS:HD3	2:B:346:TRP:CG	2.39	0.56
1:K:181:VAL:HB	2:L:352:LYS:CE	2.35	0.56
1:A:260:VAL:HB	2:P:407:TRP:CE2	2.40	0.55
1:A:397:LEU:CB	2:B:346:TRP:O	2.51	0.55
1:C:210:TYR:CD2	2:D:326:LYS:CG	2.85	0.55
1:E:177:VAL:HG11	2:F:329:ASP:CB	2.36	0.55
1:O:397:LEU:HD13	2:P:345:GLU:O	2.05	0.55
2:P:306:ASP:C	2:P:306:ASP:OD1	2.40	0.55
1:A:407:TRP:CZ2	2:B:260:VAL:HB	2.41	0.55
1:E:177:VAL:HG11	2:F:329:ASP:OD1	2.07	0.55
1:G:407:TRP:NE1	2:H:260:VAL:HB	2.21	0.55
1:M:210:TYR:CB	2:N:326:LYS:CD	2.73	0.55
2:B:407:TRP:CZ2	1:I:256:GLN:O	2.59	0.55
1:C:243:ARG:HH22	2:N:71:GLU:CD	2.10	0.55
1:C:326:LYS:CB	2:N:210:TYR:CE2	2.88	0.55
2:F:210:TYR:CE2	1:K:326:LYS:CB	2.89	0.55
1:K:177:VAL:HG11	2:L:329:ASP:OD1	2.07	0.55
1:M:407:TRP:CE3	2:N:257:VAL:HG22	2.42	0.55
1:Q:397:LEU:HB2	2:R:348:PRO:HD3	1.86	0.55
1:A:407:TRP:CE3	2:B:257:VAL:HG22	2.41	0.55
1:E:348:PRO:HD2	2:R:398:MET:HG2	1.89	0.55
1:G:401:LYS:HG2	2:H:346:TRP:CD2	2.41	0.55
1:M:181:VAL:HG11	2:N:258:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:394:LYS:CG	2:R:348:PRO:HB2	2.29	0.55
1:A:260:VAL:CB	2:P:407:TRP:CZ2	2.80	0.55
2:B:306:ASP:C	2:B:306:ASP:OD1	2.40	0.55
2:D:177:VAL:HG21	1:G:329:ASN:CG	2.26	0.55
1:E:97:GLU:CD	2:F:2:ARG:HE	1.99	0.55
1:I:100:ALA:C	2:J:254:LYS:CD	2.74	0.55
1:Q:101:ASN:CB	2:R:254:LYS:CD	2.79	0.55
1:A:256:GLN:HG2	2:P:407:TRP:CZ2	2.42	0.55
1:E:181:VAL:HG12	2:F:258:ASN:OD1	2.07	0.55
3:G:501:GTP:O1A	2:H:249:ASN:HB3	2.07	0.55
1:K:177:VAL:HB	2:L:329:ASP:HB3	1.87	0.55
1:M:283:HIS:C	1:O:56:THR:CG2	2.74	0.55
1:A:181:VAL:N	2:B:352:LYS:CE	2.62	0.55
1:C:177:VAL:HG21	2:D:329:ASP:HB3	1.89	0.55
1:I:401:LYS:CG	2:J:346:TRP:CB	2.63	0.55
1:K:176:GLN:OE1	2:L:333:LEU:CD1	2.48	0.55
1:K:407:TRP:CE2	2:L:260:VAL:HB	2.42	0.55
1:M:283:HIS:HB3	1:O:62:VAL:CG2	2.36	0.55
1:Q:97:GLU:OE2	2:R:2:ARG:N	2.40	0.55
1:C:394:LYS:HZ3	2:D:349:ASN:ND2	2.05	0.55
2:D:400:ARG:HH22	1:G:345:ASP:CG	2.10	0.55
1:I:176:GLN:HG3	2:J:333:LEU:CD2	2.33	0.55
1:I:397:LEU:HB3	2:J:346:TRP:C	2.26	0.55
1:M:100:ALA:CA	2:N:254:LYS:HD2	2.37	0.55
1:Q:404:PHE:CZ	2:R:314:THR:HG22	2.28	0.55
1:Q:406:HIS:HE1	2:R:260:VAL:HG12	1.60	0.55
1:A:176:GLN:OE1	2:B:333:LEU:CD1	2.48	0.55
1:A:326:LYS:HB2	2:P:210:TYR:HE2	1.69	0.55
1:E:210:TYR:CD1	2:F:326:LYS:CB	2.79	0.55
1:E:260:VAL:HB	2:R:407:TRP:CE2	2.40	0.55
1:M:403:ALA:HB1	2:N:261:PRO:HB3	1.87	0.55
1:E:407:TRP:HE1	2:F:260:VAL:HB	1.71	0.55
1:G:401:LYS:CG	2:H:346:TRP:CB	2.62	0.55
1:I:181:VAL:HB	2:J:352:LYS:CG	2.37	0.55
1:M:101:ASN:ND2	2:N:258:ASN:OD1	2.40	0.55
2:D:398:MET:SD	1:G:348:PRO:HG3	2.47	0.54
1:E:407:TRP:CE3	2:F:257:VAL:HG22	2.42	0.54
1:G:397:LEU:HB2	2:H:348:PRO:HD3	1.89	0.54
2:J:306:ASP:C	2:J:306:ASP:OD1	2.40	0.54
1:O:176:GLN:HB3	2:P:333:LEU:HD13	1.88	0.54
1:A:101:ASN:CA	2:B:254:LYS:CE	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HA	2:P:177:VAL:CG2	2.37	0.54
2:B:404:PHE:CE2	1:I:258:ASN:O	2.60	0.54
1:C:256:GLN:O	2:N:407:TRP:CE2	2.60	0.54
1:C:407:TRP:CE3	2:D:257:VAL:HG22	2.41	0.54
2:D:71:GLU:CD	1:G:243:ARG:HH22	2.11	0.54
2:F:177:VAL:HG21	1:K:329:ASN:CB	2.38	0.54
2:F:398:MET:SD	1:K:348:PRO:HG3	2.48	0.54
1:G:179:THR:HG21	2:H:248:LEU:CD1	2.38	0.54
1:I:179:THR:HG21	2:J:248:LEU:CD1	2.38	0.54
1:A:325:PRO:HB2	2:P:210:TYR:OH	2.06	0.54
1:A:348:PRO:CD	2:P:398:MET:HG3	2.28	0.54
1:A:407:TRP:CB	2:B:257:VAL:HG13	2.37	0.54
1:C:177:VAL:HG11	2:D:329:ASP:CB	2.38	0.54
1:C:407:TRP:CE2	2:D:260:VAL:HB	2.43	0.54
2:D:181:VAL:HA	1:G:350:GLY:CA	2.35	0.54
1:Q:401:LYS:HG2	2:R:346:TRP:CD2	2.43	0.54
1:A:346:TRP:CB	2:P:401:ARG:HB2	2.15	0.54
1:C:260:VAL:HB	2:N:407:TRP:HZ2	1.64	0.54
2:D:404:PHE:HZ	1:G:258:ASN:O	1.90	0.54
1:I:176:GLN:O	2:J:333:LEU:HD13	2.08	0.54
1:I:407:TRP:CD1	2:J:257:VAL:O	2.61	0.54
1:M:177:VAL:HG11	2:N:329:ASP:CB	2.38	0.54
1:A:283:HIS:CA	1:E:56:THR:CG2	2.78	0.54
1:A:397:LEU:HB3	2:B:346:TRP:C	2.27	0.54
2:D:407:TRP:CZ2	1:G:256:GLN:HG2	2.42	0.54
1:I:401:LYS:HG2	2:J:346:TRP:CD2	2.43	0.54
1:Q:401:LYS:CG	2:R:346:TRP:CB	2.68	0.54
1:Q:407:TRP:CE3	2:R:257:VAL:HG22	2.42	0.54
1:A:62:VAL:CG2	1:C:283:HIS:HB3	2.37	0.54
1:C:176:GLN:OE1	2:D:333:LEU:CD1	2.49	0.54
1:I:407:TRP:HE1	2:J:260:VAL:HB	1.73	0.54
1:M:283:HIS:C	1:O:56:THR:HG21	2.28	0.54
1:M:404:PHE:HE2	2:N:258:ASN:C	2.11	0.54
1:G:73:THR:HG21	2:H:245:PRO:HA	1.90	0.54
1:K:177:VAL:CB	2:L:329:ASP:HB3	2.38	0.54
1:M:179:THR:HG21	2:N:248:LEU:CD1	2.38	0.54
1:M:401:LYS:CG	2:N:346:TRP:CB	2.68	0.54
1:O:176:GLN:O	2:P:333:LEU:HD13	2.07	0.54
2:R:228:ASN:ND2	5:R:901:GDP:HN1	1.98	0.54
2:F:177:VAL:HG21	1:K:329:ASN:CG	2.28	0.53
2:F:228:ASN:ND2	5:F:901:GDP:HN1	1.98	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:TYR:CE1	2:L:326:LYS:CA	2.83	0.53
2:L:228:ASN:ND2	5:L:901:GDP:HN1	1.98	0.53
1:O:105:ARG:NE	2:P:253:ARG:HE	2.05	0.53
2:R:306:ASP:C	2:R:306:ASP:OD1	2.40	0.53
1:E:260:VAL:CB	2:R:407:TRP:CZ2	2.80	0.53
1:G:177:VAL:HG21	2:H:329:ASP:HB3	1.90	0.53
1:G:404:PHE:CZ	2:H:314:THR:HG22	2.37	0.53
1:K:210:TYR:CG	2:L:326:LYS:CB	2.91	0.53
1:M:404:PHE:CE2	2:N:258:ASN:C	2.81	0.53
1:M:407:TRP:CG	2:N:257:VAL:HA	2.43	0.53
1:Q:72:PRO:HB2	2:R:48:ARG:NH1	2.24	0.53
1:Q:101:ASN:CB	2:R:254:LYS:HG3	2.38	0.53
2:D:210:TYR:CE2	1:G:326:LYS:CB	2.89	0.53
1:O:101:ASN:ND2	2:P:258:ASN:OD1	2.41	0.53
1:A:72:PRO:HB2	2:B:48:ARG:NH1	2.24	0.53
1:M:176:GLN:O	2:N:333:LEU:HD13	2.08	0.53
1:O:179:THR:HG21	2:P:353:THR:HG1	1.68	0.53
1:O:407:TRP:HB3	2:P:257:VAL:HG13	1.89	0.53
2:B:210:TYR:CE2	1:I:326:LYS:CB	2.88	0.53
2:D:407:TRP:CZ2	1:G:256:GLN:O	2.62	0.53
2:H:345:GLU:H	2:H:345:GLU:CD	2.10	0.53
1:I:101:ASN:HB2	2:J:254:LYS:HG3	1.89	0.53
2:L:306:ASP:OD1	2:L:306:ASP:C	2.40	0.53
1:M:105:ARG:HH22	2:N:253:ARG:NH2	2.01	0.53
1:M:283:HIS:O	1:O:62:VAL:HG21	2.08	0.53
1:O:72:PRO:HB2	2:P:48:ARG:HH12	1.72	0.53
1:O:407:TRP:CZ2	2:P:260:VAL:HB	2.44	0.53
1:Q:181:VAL:HB	2:R:352:LYS:CG	2.37	0.53
2:B:398:MET:HG2	1:I:348:PRO:HD2	1.91	0.53
1:C:101:ASN:CA	2:D:254:LYS:HE3	2.33	0.53
1:E:325:PRO:HB2	2:R:210:TYR:OH	2.08	0.53
1:G:210:TYR:HB3	2:H:326:LYS:HE2	1.89	0.53
1:K:216:ASN:HB3	1:K:275:VAL:O	2.09	0.53
1:M:388:TRP:HA	1:M:388:TRP:CE3	2.44	0.53
1:Q:216:ASN:HB3	1:Q:275:VAL:O	2.09	0.53
1:Q:401:LYS:CD	2:R:346:TRP:CD2	2.91	0.53
1:A:101:ASN:HD22	2:B:258:ASN:ND2	2.07	0.53
1:A:179:THR:HG21	2:B:248:LEU:CD1	2.39	0.53
1:C:210:TYR:CG	2:D:326:LYS:HB2	2.40	0.53
1:C:388:TRP:CE3	1:C:388:TRP:HA	2.44	0.53
2:D:345:GLU:H	2:D:345:GLU:CD	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ASN:HD22	2:F:258:ASN:HD21	1.56	0.53
1:E:181:VAL:HB	2:F:352:LYS:CE	2.37	0.53
1:E:216:ASN:HB3	1:E:275:VAL:O	2.09	0.53
2:F:181:VAL:HA	1:K:350:GLY:CA	2.37	0.53
1:G:176:GLN:HG3	2:H:333:LEU:CD2	2.36	0.53
1:G:388:TRP:HA	1:G:388:TRP:CE3	2.44	0.53
2:H:228:ASN:ND2	5:H:901:GDP:HN1	1.98	0.53
1:K:401:LYS:HZ3	2:L:346:TRP:HE1	1.57	0.53
1:K:407:TRP:HE1	2:L:260:VAL:HB	1.74	0.53
1:M:271:THR:OG1	1:M:301:GLN:NE2	2.42	0.53
1:O:210:TYR:CD1	2:P:326:LYS:HD2	2.44	0.53
1:Q:179:THR:CB	2:R:353:THR:H	2.22	0.53
1:A:216:ASN:HB3	1:A:275:VAL:O	2.09	0.53
1:A:407:TRP:CG	2:B:257:VAL:HG13	2.43	0.53
1:C:397:LEU:CB	2:D:346:TRP:O	2.55	0.53
1:E:101:ASN:CA	2:F:254:LYS:HE3	2.31	0.53
2:F:306:ASP:C	2:F:306:ASP:OD1	2.40	0.53
1:G:176:GLN:O	2:H:333:LEU:HD13	2.09	0.53
1:G:181:VAL:HB	2:H:352:LYS:CG	2.39	0.53
1:G:271:THR:OG1	1:G:301:GLN:NE2	2.42	0.53
2:H:221:THR:H	2:H:222:PRO:HD3	1.73	0.53
1:I:404:PHE:HE2	2:J:258:ASN:C	2.12	0.53
1:M:100:ALA:CB	2:N:254:LYS:HB2	2.39	0.53
1:M:407:TRP:CG	2:N:257:VAL:HG13	2.44	0.53
1:O:216:ASN:HB3	1:O:275:VAL:O	2.09	0.53
1:A:401:LYS:CG	2:B:346:TRP:CD2	2.92	0.53
1:C:345:ASP:OD1	2:N:400:ARG:NH2	2.39	0.53
2:D:221:THR:H	2:D:222:PRO:HD3	1.73	0.53
2:D:404:PHE:CE2	1:G:258:ASN:HA	2.44	0.53
1:E:326:LYS:HB2	2:R:210:TYR:HE2	1.71	0.53
1:G:283:HIS:O	1:I:62:VAL:HG21	2.08	0.53
1:I:210:TYR:OH	2:J:326:LYS:HA	2.06	0.53
2:N:221:THR:H	2:N:222:PRO:HD3	1.73	0.53
2:N:345:GLU:H	2:N:345:GLU:CD	2.10	0.53
1:O:401:LYS:HE3	2:P:435:TYR:HD2	1.74	0.53
1:Q:100:ALA:HA	2:R:254:LYS:HD2	1.91	0.53
1:Q:176:GLN:HG3	2:R:333:LEU:CD2	2.28	0.53
1:Q:177:VAL:HG11	2:R:329:ASP:CB	2.38	0.53
1:Q:394:LYS:CB	2:R:348:PRO:HG3	2.38	0.53
1:Q:401:LYS:HG2	2:R:346:TRP:CG	2.41	0.53
1:C:271:THR:OG1	1:C:301:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:TRP:CG	2:D:257:VAL:HG13	2.44	0.52
1:E:100:ALA:HA	2:F:254:LYS:HD2	1.90	0.52
1:E:271:THR:OG1	1:E:301:GLN:NE2	2.42	0.52
1:E:388:TRP:HA	1:E:388:TRP:CE3	2.44	0.52
1:G:283:HIS:HB3	1:I:62:VAL:CG2	2.38	0.52
1:I:216:ASN:HB3	1:I:275:VAL:O	2.09	0.52
1:K:271:THR:OG1	1:K:301:GLN:NE2	2.42	0.52
1:M:177:VAL:CB	2:N:329:ASP:HB3	2.38	0.52
1:O:388:TRP:HA	1:O:388:TRP:CE3	2.44	0.52
1:A:177:VAL:HG11	2:B:329:ASP:CB	2.38	0.52
2:B:221:THR:H	2:B:222:PRO:HD3	1.73	0.52
2:D:228:ASN:ND2	5:D:901:GDP:HN1	1.98	0.52
1:I:72:PRO:HB2	2:J:48:ARG:NH1	2.25	0.52
1:I:394:LYS:C	2:J:348:PRO:HG3	2.29	0.52
2:J:221:THR:H	2:J:222:PRO:HD3	1.73	0.52
1:M:407:TRP:CD1	2:N:257:VAL:O	2.62	0.52
1:O:394:LYS:CB	2:P:348:PRO:CG	2.88	0.52
2:P:221:THR:H	2:P:222:PRO:HD3	1.73	0.52
1:Q:271:THR:OG1	1:Q:301:GLN:NE2	2.42	0.52
1:Q:388:TRP:HA	1:Q:388:TRP:CE3	2.44	0.52
1:A:283:HIS:O	1:E:62:VAL:HG21	2.08	0.52
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.44	0.52
1:C:216:ASN:HB3	1:C:275:VAL:O	2.09	0.52
2:F:306:ASP:OD1	2:F:308:ARG:HG2	2.09	0.52
1:I:210:TYR:CB	2:J:326:LYS:CD	2.73	0.52
2:L:306:ASP:OD1	2:L:308:ARG:HG2	2.10	0.52
1:M:101:ASN:ND2	2:N:258:ASN:HD21	2.07	0.52
1:M:216:ASN:HB3	1:M:275:VAL:O	2.09	0.52
1:O:407:TRP:CH2	2:P:256:ALA:HB1	2.44	0.52
2:P:283:TYR:HD2	2:R:62:VAL:CG2	2.07	0.52
1:Q:100:ALA:CA	2:R:254:LYS:CB	2.73	0.52
2:R:306:ASP:OD1	2:R:308:ARG:HG2	2.09	0.52
1:A:73:THR:HG21	2:B:245:PRO:HA	1.92	0.52
1:A:394:LYS:HZ3	2:B:349:ASN:ND2	2.05	0.52
2:B:56:ALA:HB2	2:D:283:TYR:C	2.28	0.52
1:G:216:ASN:HB3	1:G:275:VAL:O	2.09	0.52
1:G:407:TRP:CD1	2:H:257:VAL:O	2.63	0.52
1:I:388:TRP:HA	1:I:388:TRP:CE3	2.44	0.52
1:K:388:TRP:CE3	1:K:388:TRP:HA	2.44	0.52
1:M:406:HIS:NE2	2:N:260:VAL:HG11	2.21	0.52
1:Q:407:TRP:CG	2:R:257:VAL:HG13	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASP:OD1	2:B:308:ARG:HG2	2.09	0.52
2:B:404:PHE:CE2	1:I:258:ASN:HA	2.44	0.52
1:C:260:VAL:CB	2:N:407:TRP:CZ2	2.84	0.52
2:F:400:ARG:HH22	1:K:345:ASP:CG	2.12	0.52
1:I:97:GLU:OE2	2:J:2:ARG:N	2.43	0.52
2:N:228:ASN:ND2	5:N:901:GDP:HN1	1.98	0.52
2:P:306:ASP:OD1	2:P:308:ARG:HG2	2.09	0.52
1:Q:181:VAL:HG11	2:R:258:ASN:O	2.08	0.52
1:A:348:PRO:HG3	2:P:398:MET:CG	2.40	0.52
1:A:407:TRP:CE2	2:B:260:VAL:HB	2.44	0.52
1:E:176:GLN:O	2:F:333:LEU:HD13	2.10	0.52
2:F:221:THR:H	2:F:222:PRO:HD3	1.73	0.52
1:I:179:THR:HA	2:J:353:THR:N	2.22	0.52
1:I:271:THR:OG1	1:I:301:GLN:NE2	2.42	0.52
2:P:10:GLY:HA2	2:P:145:THR:OG1	2.10	0.52
1:A:62:VAL:HG21	1:C:283:HIS:O	2.09	0.52
1:A:177:VAL:CG1	2:B:329:ASP:HA	2.28	0.52
1:A:256:GLN:O	2:P:407:TRP:NE1	2.43	0.52
1:C:346:TRP:HZ3	2:N:403:ALA:CB	1.85	0.52
1:E:407:TRP:CB	2:F:257:VAL:HG13	2.40	0.52
2:J:221:THR:N	2:J:222:PRO:CD	2.73	0.52
1:K:101:ASN:HB2	2:L:254:LYS:HG3	1.91	0.52
1:M:105:ARG:NE	2:N:253:ARG:HE	2.07	0.52
1:Q:177:VAL:HG11	2:R:329:ASP:OD1	2.09	0.52
1:A:271:THR:OG1	1:A:301:GLN:NE2	2.42	0.52
1:A:401:LYS:CD	2:B:346:TRP:CD2	2.89	0.52
2:B:221:THR:N	2:B:222:PRO:CD	2.73	0.52
1:C:407:TRP:CB	2:D:257:VAL:HG13	2.39	0.52
2:D:10:GLY:HA2	2:D:145:THR:OG1	2.10	0.52
2:J:306:ASP:OD1	2:J:308:ARG:HG2	2.10	0.52
2:L:221:THR:H	2:L:222:PRO:HD3	1.73	0.52
1:M:397:LEU:C	2:N:346:TRP:O	2.48	0.52
1:O:100:ALA:HA	2:P:254:LYS:HD2	1.92	0.52
1:O:271:THR:OG1	1:O:301:GLN:NE2	2.42	0.52
1:O:401:LYS:HG2	2:P:346:TRP:CD2	2.45	0.52
2:P:221:THR:N	2:P:222:PRO:CD	2.73	0.52
1:Q:100:ALA:CB	2:R:254:LYS:HB2	2.40	0.52
2:R:10:GLY:HA2	2:R:145:THR:OG1	2.10	0.52
1:A:176:GLN:HB3	2:B:333:LEU:HD13	1.92	0.52
1:C:179:THR:HG21	2:D:248:LEU:CD1	2.40	0.52
1:E:407:TRP:NE1	2:F:260:VAL:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:TYR:CG	2:L:326:LYS:HB2	2.37	0.52
1:K:397:LEU:CB	2:L:346:TRP:O	2.58	0.52
1:M:394:LYS:CB	2:N:348:PRO:HG3	2.39	0.52
1:M:401:LYS:CG	2:N:346:TRP:CD2	2.93	0.52
2:N:10:GLY:HA2	2:N:145:THR:OG1	2.10	0.52
1:O:401:LYS:CG	2:P:346:TRP:CD2	2.92	0.52
2:B:10:GLY:HA2	2:B:145:THR:OG1	2.10	0.52
2:B:401:ARG:NH2	1:I:435:VAL:HG22	2.25	0.52
2:F:10:GLY:HA2	2:F:145:THR:OG1	2.10	0.52
2:F:210:TYR:HE2	1:K:326:LYS:HB2	1.73	0.52
1:G:101:ASN:HB2	2:H:254:LYS:HG3	1.91	0.52
2:H:10:GLY:HA2	2:H:145:THR:OG1	2.10	0.52
1:I:101:ASN:HD22	2:J:258:ASN:ND2	2.08	0.52
2:J:10:GLY:HA2	2:J:145:THR:OG1	2.10	0.52
2:L:10:GLY:HA2	2:L:145:THR:OG1	2.10	0.52
1:Q:403:ALA:HB1	2:R:261:PRO:HB3	1.91	0.52
1:A:177:VAL:HG21	2:B:329:ASP:HB3	1.90	0.51
1:A:325:PRO:HG2	2:P:224:TYR:CE1	2.45	0.51
1:A:346:TRP:CA	2:P:401:ARG:HG3	2.32	0.51
2:H:306:ASP:OD1	2:H:308:ARG:HG2	2.09	0.51
1:M:100:ALA:C	2:N:254:LYS:CG	2.78	0.51
2:R:221:THR:H	2:R:222:PRO:HD3	1.73	0.51
1:A:397:LEU:HD22	2:B:345:GLU:O	2.10	0.51
2:D:221:THR:N	2:D:222:PRO:CD	2.73	0.51
1:I:407:TRP:CE2	2:J:260:VAL:HB	2.45	0.51
1:K:407:TRP:CD1	2:L:257:VAL:O	2.63	0.51
2:N:221:THR:N	2:N:222:PRO:CD	2.73	0.51
1:Q:407:TRP:CD1	2:R:257:VAL:O	2.62	0.51
2:B:210:TYR:HE2	1:I:326:LYS:HB2	1.72	0.51
1:C:388:TRP:HA	1:C:388:TRP:HE3	1.74	0.51
1:E:407:TRP:CG	2:F:257:VAL:HG13	2.45	0.51
2:H:390:ARG:HA	2:H:390:ARG:NE	2.26	0.51
1:M:388:TRP:HA	1:M:388:TRP:HE3	1.74	0.51
1:C:260:VAL:HB	2:N:407:TRP:CE2	2.44	0.51
1:G:388:TRP:HA	1:G:388:TRP:HE3	1.74	0.51
2:H:221:THR:N	2:H:222:PRO:CD	2.73	0.51
1:M:401:LYS:HG2	2:N:346:TRP:CG	2.43	0.51
1:O:394:LYS:CB	2:P:348:PRO:HG3	2.39	0.51
1:A:258:ASN:CA	2:P:404:PHE:CE2	2.93	0.51
1:A:329:ASN:HB2	2:P:177:VAL:HG21	1.92	0.51
1:C:101:ASN:CA	2:D:254:LYS:CE	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ARG:NE	2:D:390:ARG:HA	2.26	0.51
2:J:390:ARG:NE	2:J:390:ARG:HA	2.26	0.51
1:M:394:LYS:CG	2:N:348:PRO:HB2	2.30	0.51
1:Q:100:ALA:C	2:R:254:LYS:CG	2.78	0.51
2:B:407:TRP:CZ2	1:I:256:GLN:HG2	2.46	0.51
1:C:177:VAL:CG1	2:D:329:ASP:HA	2.29	0.51
2:D:306:ASP:OD1	2:D:308:ARG:HG2	2.10	0.51
1:E:100:ALA:CA	2:F:254:LYS:HD2	2.41	0.51
3:E:501:GTP:O1A	2:F:249:ASN:HB3	2.10	0.51
1:G:181:VAL:N	2:H:352:LYS:CE	2.55	0.51
1:I:210:TYR:CD2	2:J:326:LYS:CB	2.94	0.51
1:I:397:LEU:CB	2:J:346:TRP:O	2.54	0.51
1:I:404:PHE:CZ	2:J:314:THR:HG22	2.35	0.51
1:K:100:ALA:HA	2:L:254:LYS:CD	2.40	0.51
2:L:221:THR:N	2:L:222:PRO:CD	2.73	0.51
2:N:390:ARG:NE	2:N:390:ARG:HA	2.26	0.51
1:O:388:TRP:HA	1:O:388:TRP:HE3	1.74	0.51
1:Q:210:TYR:CD1	2:R:326:LYS:HD2	2.46	0.51
1:A:348:PRO:HG3	2:P:398:MET:HG3	1.93	0.51
2:B:404:PHE:HZ	1:I:258:ASN:O	1.91	0.51
1:G:100:ALA:C	2:H:254:LYS:CD	2.77	0.51
1:G:407:TRP:CE2	2:H:260:VAL:HB	2.46	0.51
1:I:181:VAL:HB	2:J:352:LYS:CE	2.37	0.51
2:N:306:ASP:OD1	2:N:308:ARG:HG2	2.10	0.51
1:Q:406:HIS:HE1	2:R:260:VAL:C	2.11	0.51
1:C:397:LEU:HD22	2:D:345:GLU:O	2.11	0.51
1:G:237:SER:O	1:G:241:SER:OG	2.29	0.51
1:I:105:ARG:HH22	2:J:253:ARG:NH2	2.04	0.51
1:K:397:LEU:HB3	2:L:346:TRP:C	2.30	0.51
2:L:390:ARG:NE	2:L:390:ARG:HA	2.26	0.51
1:M:401:LYS:HE3	2:N:435:TYR:HD2	1.76	0.51
2:B:390:ARG:NE	2:B:390:ARG:HA	2.26	0.51
1:C:237:SER:O	1:C:241:SER:OG	2.29	0.51
2:F:221:THR:N	2:F:222:PRO:CD	2.73	0.51
2:F:390:ARG:NE	2:F:390:ARG:HA	2.26	0.51
1:M:406:HIS:HE1	2:N:260:VAL:C	2.10	0.51
1:O:407:TRP:CZ2	2:P:256:ALA:C	2.83	0.51
2:P:390:ARG:HA	2:P:390:ARG:NE	2.26	0.51
1:C:397:LEU:HB3	2:D:346:TRP:C	2.31	0.51
1:K:397:LEU:HB2	2:L:348:PRO:HD3	1.93	0.51
1:M:179:THR:CB	2:N:353:THR:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:177:VAL:CB	2:R:329:ASP:HB3	2.41	0.51
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.74	0.50
1:G:397:LEU:HB3	2:H:346:TRP:C	2.30	0.50
1:G:407:TRP:HE1	2:H:260:VAL:HB	1.76	0.50
2:H:283:TYR:HD2	2:J:62:VAL:CG2	2.03	0.50
1:K:210:TYR:CD1	2:L:326:LYS:HD2	2.46	0.50
1:M:237:SER:O	1:M:241:SER:OG	2.29	0.50
1:O:179:THR:CB	2:P:353:THR:H	2.24	0.50
1:Q:406:HIS:NE2	2:R:260:VAL:HG11	2.23	0.50
1:E:256:GLN:CG	2:R:407:TRP:CH2	2.92	0.50
1:G:97:GLU:OE2	2:H:2:ARG:N	2.44	0.50
3:K:501:GTP:O1A	2:L:249:ASN:HB3	2.10	0.50
2:R:221:THR:N	2:R:222:PRO:CD	2.73	0.50
1:E:388:TRP:HA	1:E:388:TRP:HE3	1.74	0.50
1:E:394:LYS:O	2:F:348:PRO:HG3	2.11	0.50
1:I:237:SER:O	1:I:241:SER:OG	2.29	0.50
1:I:388:TRP:HA	1:I:388:TRP:HE3	1.74	0.50
1:M:394:LYS:CB	2:N:348:PRO:CG	2.89	0.50
2:R:390:ARG:NE	2:R:390:ARG:HA	2.26	0.50
1:A:237:SER:O	1:A:241:SER:OG	2.29	0.50
1:E:73:THR:HG21	2:F:245:PRO:HA	1.94	0.50
1:M:401:LYS:HG2	2:N:346:TRP:CD2	2.47	0.50
1:Q:237:SER:O	1:Q:241:SER:OG	2.29	0.50
1:Q:388:TRP:HA	1:Q:388:TRP:HE3	1.74	0.50
1:Q:394:LYS:CB	2:R:348:PRO:CG	2.89	0.50
1:A:210:TYR:CG	2:B:326:LYS:HB2	2.39	0.50
1:C:329:ASN:HA	2:N:177:VAL:CG2	2.42	0.50
1:I:177:VAL:HG21	2:J:329:ASP:HB3	1.93	0.50
1:Q:100:ALA:C	2:R:254:LYS:CD	2.74	0.50
1:Q:407:TRP:CG	2:R:257:VAL:HA	2.46	0.50
1:C:348:PRO:CG	2:N:398:MET:CG	2.89	0.50
1:E:258:ASN:O	2:R:404:PHE:HZ	1.92	0.50
1:G:177:VAL:CG2	2:H:329:ASP:HB3	2.42	0.50
1:I:100:ALA:CB	2:J:254:LYS:HB2	2.41	0.50
1:I:210:TYR:CD1	2:J:326:LYS:HD2	2.47	0.50
1:K:388:TRP:HA	1:K:388:TRP:HE3	1.74	0.50
1:K:394:LYS:C	2:L:348:PRO:HG3	2.31	0.50
1:O:237:SER:O	1:O:241:SER:OG	2.29	0.50
1:A:397:LEU:HB2	2:B:348:PRO:HD3	1.94	0.50
1:C:346:TRP:CB	2:N:401:ARG:HB2	2.22	0.50
2:D:404:PHE:HE2	1:G:258:ASN:CA	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:SER:O	1:E:241:SER:OG	2.29	0.50
1:O:101:ASN:ND2	2:P:258:ASN:HD21	2.05	0.50
1:C:258:ASN:CA	2:N:404:PHE:CE2	2.94	0.50
2:F:407:TRP:CZ2	1:K:256:GLN:HG2	2.46	0.50
1:I:100:ALA:HA	2:J:254:LYS:CD	2.42	0.50
1:A:2:ARG:N	2:P:96:GLN:NE2	2.60	0.50
1:C:181:VAL:HB	2:D:352:LYS:CE	2.42	0.50
1:E:101:ASN:CA	2:F:254:LYS:CE	2.90	0.50
1:E:258:ASN:HA	2:R:404:PHE:CE2	2.46	0.50
1:G:177:VAL:HG21	2:H:329:ASP:CB	2.42	0.50
2:N:12:CYS:SG	2:N:13:GLY:N	2.85	0.50
2:D:404:PHE:CE2	1:G:258:ASN:O	2.64	0.49
1:E:345:ASP:OD1	2:R:400:ARG:NH2	2.42	0.49
1:G:210:TYR:OH	2:H:326:LYS:CA	2.53	0.49
1:G:210:TYR:CB	2:H:326:LYS:CD	2.76	0.49
1:G:404:PHE:HE2	2:H:258:ASN:C	2.14	0.49
2:H:12:CYS:SG	2:H:13:GLY:N	2.85	0.49
1:I:407:TRP:HB3	2:J:257:VAL:HG13	1.93	0.49
1:K:176:GLN:HB3	2:L:333:LEU:HD13	1.94	0.49
1:Q:397:LEU:C	2:R:346:TRP:O	2.49	0.49
1:C:101:ASN:HD22	2:D:258:ASN:ND2	2.10	0.49
2:D:12:CYS:SG	2:D:13:GLY:N	2.86	0.49
1:K:181:VAL:HB	2:L:352:LYS:CG	2.41	0.49
1:K:237:SER:O	1:K:241:SER:OG	2.29	0.49
1:K:404:PHE:CZ	2:L:314:THR:HG22	2.35	0.49
1:K:407:TRP:HB3	2:L:257:VAL:HG13	1.94	0.49
2:L:2:ARG:N	2:L:131:CYS:O	2.45	0.49
1:M:100:ALA:HA	2:N:254:LYS:HD2	1.94	0.49
1:O:181:VAL:N	2:P:352:LYS:CD	2.75	0.49
2:B:404:PHE:HE2	1:I:258:ASN:CA	2.25	0.49
1:E:177:VAL:HG21	2:F:329:ASP:HB3	1.93	0.49
1:E:256:GLN:HG2	2:R:407:TRP:CZ2	2.47	0.49
2:J:2:ARG:N	2:J:131:CYS:O	2.45	0.49
1:M:210:TYR:CD2	2:N:326:LYS:CB	2.95	0.49
1:O:100:ALA:C	2:P:254:LYS:HG3	2.33	0.49
1:O:105:ARG:HH22	2:P:253:ARG:CZ	2.20	0.49
1:A:404:PHE:HE2	2:B:258:ASN:C	2.15	0.49
1:C:176:GLN:HB3	2:D:333:LEU:HD13	1.94	0.49
1:C:177:VAL:CB	2:D:329:ASP:HB3	2.43	0.49
2:F:2:ARG:N	2:F:131:CYS:O	2.45	0.49
1:O:283:HIS:O	1:Q:62:VAL:HG21	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:N	2:B:131:CYS:O	2.45	0.49
2:B:283:TYR:CA	2:F:56:ALA:HB2	2.38	0.49
1:C:181:VAL:N	2:D:352:LYS:CE	2.61	0.49
1:E:397:LEU:HD22	2:F:345:GLU:O	2.13	0.49
1:I:181:VAL:CG2	2:J:352:LYS:HE2	2.41	0.49
1:I:401:LYS:HZ3	2:J:346:TRP:HE1	1.56	0.49
2:J:12:CYS:SG	2:J:13:GLY:N	2.85	0.49
2:N:2:ARG:N	2:N:131:CYS:O	2.45	0.49
2:P:282:GLN:O	2:R:60:LYS:CG	2.61	0.49
1:Q:407:TRP:HB3	2:R:257:VAL:HG13	1.93	0.49
2:R:96:GLN:NE2	2:R:96:GLN:O	2.46	0.49
1:E:256:GLN:O	2:R:407:TRP:CE2	2.65	0.49
2:F:96:GLN:NE2	2:F:96:GLN:O	2.46	0.49
2:F:404:PHE:CE2	1:K:258:ASN:HA	2.47	0.49
1:G:181:VAL:CG2	2:H:352:LYS:HE2	2.42	0.49
2:J:228:ASN:ND2	5:J:901:GDP:HN1	1.98	0.49
2:R:2:ARG:N	2:R:131:CYS:O	2.45	0.49
2:R:12:CYS:SG	2:R:13:GLY:N	2.85	0.49
2:B:12:CYS:SG	2:B:13:GLY:N	2.85	0.49
2:B:228:ASN:ND2	5:B:901:GDP:HN1	1.98	0.49
1:C:2:ARG:N	2:N:96:GLN:NE2	2.61	0.49
2:D:2:ARG:N	2:D:131:CYS:O	2.45	0.49
1:E:101:ASN:ND2	2:F:258:ASN:OD1	2.45	0.49
1:E:177:VAL:CG1	2:F:329:ASP:HA	2.30	0.49
1:E:404:PHE:CZ	2:F:314:THR:HG22	2.38	0.49
2:F:12:CYS:SG	2:F:13:GLY:N	2.85	0.49
1:G:210:TYR:CD2	2:H:326:LYS:CB	2.96	0.49
1:G:397:LEU:CB	2:H:346:TRP:O	2.58	0.49
2:H:2:ARG:N	2:H:131:CYS:O	2.45	0.49
1:I:176:GLN:HB3	2:J:333:LEU:HD13	1.94	0.49
1:I:179:THR:HG22	2:J:353:THR:CB	2.32	0.49
1:K:101:ASN:HD22	2:L:258:ASN:ND2	2.11	0.49
1:K:101:ASN:ND2	2:L:258:ASN:OD1	2.46	0.49
1:K:401:LYS:CG	2:L:346:TRP:CB	2.65	0.49
2:P:2:ARG:N	2:P:131:CYS:O	2.45	0.49
1:A:404:PHE:H	2:B:261:PRO:C	2.15	0.49
2:D:96:GLN:NE2	2:D:96:GLN:O	2.46	0.49
2:H:96:GLN:NE2	2:H:96:GLN:O	2.46	0.49
2:L:12:CYS:SG	2:L:13:GLY:N	2.85	0.49
1:O:101:ASN:CA	2:P:254:LYS:CD	2.90	0.49
2:P:12:CYS:SG	2:P:13:GLY:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:TYR:CG	2:F:326:LYS:HB2	2.45	0.49
2:L:96:GLN:O	2:L:96:GLN:NE2	2.46	0.49
2:N:96:GLN:NE2	2:N:96:GLN:O	2.46	0.49
1:A:2:ARG:HG2	2:P:96:GLN:NE2	2.20	0.49
1:A:100:ALA:CA	2:B:254:LYS:HD2	2.43	0.49
1:C:401:LYS:HG2	2:D:346:TRP:CD2	2.48	0.49
2:F:407:TRP:CZ2	1:K:256:GLN:O	2.66	0.49
1:G:100:ALA:HA	2:H:254:LYS:CD	2.43	0.49
1:I:404:PHE:CE2	2:J:258:ASN:C	2.85	0.49
2:P:228:ASN:ND2	5:P:901:GDP:HN1	1.98	0.49
1:E:346:TRP:CB	2:R:401:ARG:HB2	2.22	0.48
1:O:73:THR:HG23	2:P:245:PRO:HG3	1.95	0.48
1:Q:404:PHE:HE2	2:R:258:ASN:C	2.15	0.48
1:A:101:ASN:CB	2:B:254:LYS:HG3	2.42	0.48
1:A:177:VAL:CB	2:B:329:ASP:HB3	2.43	0.48
1:A:346:TRP:HB2	2:P:401:ARG:HB3	1.85	0.48
2:B:96:GLN:NE2	2:B:96:GLN:O	2.46	0.48
1:C:100:ALA:HA	2:D:254:LYS:HD2	1.95	0.48
1:G:394:LYS:C	2:H:348:PRO:HG3	2.32	0.48
1:G:406:HIS:HE1	2:H:260:VAL:C	2.16	0.48
1:I:100:ALA:CA	2:J:254:LYS:CB	2.81	0.48
1:I:100:ALA:HB1	2:J:254:LYS:CA	2.41	0.48
2:J:96:GLN:O	2:J:96:GLN:NE2	2.46	0.48
1:M:72:PRO:HB2	2:N:48:ARG:HH12	1.76	0.48
1:G:72:PRO:HB2	2:H:48:ARG:NH1	2.28	0.48
1:I:177:VAL:CG2	2:J:329:ASP:HB3	2.44	0.48
1:M:210:TYR:CD1	2:N:326:LYS:HD2	2.49	0.48
2:P:96:GLN:NE2	2:P:96:GLN:O	2.46	0.48
2:P:282:GLN:HB3	2:R:60:LYS:HG3	1.95	0.48
1:Q:105:ARG:NE	2:R:253:ARG:HE	2.10	0.48
1:Q:394:LYS:HB3	2:R:348:PRO:CG	2.43	0.48
1:C:177:VAL:HG21	2:D:329:ASP:CB	2.44	0.48
1:C:326:LYS:HB2	2:N:210:TYR:HE2	1.72	0.48
2:F:404:PHE:HZ	1:K:258:ASN:O	1.95	0.48
1:O:181:VAL:CG2	2:P:352:LYS:HE2	2.40	0.48
1:A:260:VAL:O	2:P:406:HIS:NE2	2.38	0.48
1:C:72:PRO:HB2	2:D:48:ARG:NH1	2.29	0.48
1:C:256:GLN:O	2:N:407:TRP:NE1	2.46	0.48
1:E:258:ASN:CA	2:R:404:PHE:HE2	2.26	0.48
1:G:181:VAL:HA	2:H:352:LYS:HZ1	1.76	0.48
1:G:210:TYR:OH	2:H:326:LYS:HA	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:HIS:CA	1:K:56:THR:CG2	2.83	0.48
1:O:100:ALA:HA	2:P:254:LYS:CD	2.43	0.48
2:P:332:MET:HE1	2:P:332:MET:HA	1.96	0.48
1:Q:100:ALA:C	2:R:254:LYS:HG3	2.34	0.48
1:Q:179:THR:HG21	2:R:248:LEU:CD1	2.43	0.48
1:A:2:ARG:HD3	2:P:72:PRO:HD2	1.96	0.48
2:B:332:MET:HE1	2:B:332:MET:HA	1.96	0.48
1:C:397:LEU:HB2	2:D:348:PRO:HD3	1.96	0.48
2:D:176:LYS:HD3	1:G:333:ALA:CB	2.43	0.48
1:E:2:ARG:N	2:R:96:GLN:NE2	2.62	0.48
2:J:332:MET:HE1	2:J:332:MET:HA	1.96	0.48
1:Q:401:LYS:HE3	2:R:435:TYR:HD2	1.78	0.48
1:Q:404:PHE:CE2	2:R:258:ASN:C	2.86	0.48
1:A:210:TYR:CG	2:B:326:LYS:CB	2.97	0.48
2:D:407:TRP:CH2	1:G:256:GLN:CG	2.95	0.48
1:E:439:SER:OG	2:R:400:ARG:NH1	2.44	0.48
1:G:101:ASN:HD22	2:H:258:ASN:ND2	2.11	0.48
1:C:73:THR:HG21	2:D:245:PRO:HA	1.96	0.48
1:I:177:VAL:HG21	2:J:329:ASP:CB	2.44	0.48
2:J:288:VAL:HB	2:J:327:GLU:HG2	1.96	0.48
1:K:100:ALA:C	2:L:254:LYS:CD	2.77	0.48
1:M:407:TRP:HB3	2:N:257:VAL:HG13	1.94	0.48
2:P:288:VAL:HB	2:P:327:GLU:HG2	1.96	0.48
1:A:177:VAL:HB	2:B:329:ASP:HB3	1.95	0.48
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.96	0.48
1:C:348:PRO:CD	2:N:398:MET:HG3	2.33	0.48
1:E:97:GLU:OE2	2:F:2:ARG:N	2.47	0.48
1:G:407:TRP:HB3	2:H:257:VAL:HG13	1.95	0.48
1:A:254:GLU:HB2	2:P:100:GLY:HA2	1.95	0.47
2:B:407:TRP:CE2	1:I:260:VAL:HB	2.47	0.47
1:C:394:LYS:O	2:D:348:PRO:HG3	2.14	0.47
2:D:398:MET:HG2	1:G:348:PRO:HD2	1.96	0.47
1:E:176:GLN:HB3	2:F:333:LEU:HD13	1.96	0.47
1:O:403:ALA:HB1	2:P:261:PRO:CB	2.43	0.47
2:P:282:GLN:O	2:R:60:LYS:HG3	2.13	0.47
1:Q:224:TYR:CG	2:R:325:MET:CG	2.84	0.47
1:A:181:VAL:HB	2:B:352:LYS:CE	2.44	0.47
1:K:179:THR:HG21	2:L:248:LEU:CD1	2.44	0.47
2:B:96:GLN:NE2	1:I:2:ARG:N	2.63	0.47
1:C:177:VAL:HB	2:D:329:ASP:HB3	1.95	0.47
1:E:177:VAL:CB	2:F:329:ASP:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ASN:HA	2:R:177:VAL:CG2	2.45	0.47
1:G:177:VAL:HG11	2:H:329:ASP:CG	2.33	0.47
1:K:397:LEU:HD13	2:L:345:GLU:O	2.14	0.47
2:L:288:VAL:HB	2:L:327:GLU:HG2	1.96	0.47
1:O:224:TYR:CG	2:P:325:MET:CG	2.86	0.47
1:A:177:VAL:HG21	2:B:329:ASP:CB	2.45	0.47
2:B:283:TYR:HA	2:F:56:ALA:HB2	1.85	0.47
1:C:177:VAL:CG2	2:D:329:ASP:HB3	2.45	0.47
2:D:96:GLN:NE2	1:G:2:ARG:N	2.63	0.47
1:G:53:PHE:HB3	1:G:61:HIS:HB3	1.96	0.47
1:K:100:ALA:CB	2:L:254:LYS:HB2	2.44	0.47
1:K:210:TYR:CB	2:L:326:LYS:CD	2.78	0.47
1:O:394:LYS:HB3	2:P:348:PRO:CG	2.44	0.47
1:Q:101:ASN:ND2	2:R:258:ASN:HD21	2.10	0.47
1:A:284:GLU:N	1:E:56:THR:HG22	2.29	0.47
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.69	0.47
1:C:11:GLN:HE22	2:D:247:GLN:C	2.09	0.47
1:C:53:PHE:HB3	1:C:61:HIS:HB3	1.97	0.47
1:C:100:ALA:CA	2:D:254:LYS:HD2	2.44	0.47
1:C:210:TYR:CG	2:D:326:LYS:CB	2.98	0.47
1:C:401:LYS:HZ3	2:D:346:TRP:HE1	1.61	0.47
2:F:288:VAL:HB	2:F:327:GLU:HG2	1.96	0.47
1:M:53:PHE:HB3	1:M:61:HIS:HB3	1.97	0.47
1:M:96:LYS:O	2:N:2:ARG:NE	2.48	0.47
1:O:402:ARG:HD3	1:O:402:ARG:HA	1.69	0.47
2:R:288:VAL:HB	2:R:327:GLU:HG2	1.96	0.47
1:A:210:TYR:CE2	2:B:326:LYS:CB	2.97	0.47
2:B:400:ARG:NH2	1:I:345:ASP:OD1	2.44	0.47
1:E:101:ASN:HD22	2:F:258:ASN:ND2	2.13	0.47
1:A:210:TYR:CG	2:B:326:LYS:CD	2.98	0.47
1:E:246:GLY:HA3	1:E:356:ASN:HA	1.97	0.47
2:F:176:LYS:HD3	1:K:333:ALA:CB	2.42	0.47
2:J:282:GLN:HB3	2:L:60:LYS:HG3	1.96	0.47
1:K:105:ARG:NH2	2:L:253:ARG:HH21	1.71	0.47
1:K:246:GLY:HA3	1:K:356:ASN:HA	1.97	0.47
1:K:332:ILE:HA	1:K:335:ILE:HG12	1.97	0.47
1:O:53:PHE:HB3	1:O:61:HIS:HB3	1.97	0.47
1:O:72:PRO:CB	2:P:48:ARG:HH12	2.27	0.47
1:Q:100:ALA:HA	2:R:254:LYS:CD	2.43	0.47
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	1.96	0.47
1:G:100:ALA:CA	2:H:254:LYS:CB	2.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:PHE:HB3	1:I:61:HIS:HB3	1.97	0.47
1:K:100:ALA:HB1	2:L:254:LYS:CA	2.43	0.47
1:K:179:THR:HG22	2:L:353:THR:CB	2.36	0.47
1:M:394:LYS:HB3	2:N:348:PRO:CG	2.45	0.47
1:O:177:VAL:CG2	2:P:329:ASP:HB3	2.45	0.47
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.97	0.47
1:C:228:ASN:HD21	3:C:501:GTP:HN1	1.63	0.47
1:K:97:GLU:OE2	2:L:2:ARG:N	2.48	0.47
1:K:404:PHE:HE2	2:L:258:ASN:C	2.18	0.47
1:M:228:ASN:HD21	3:M:501:GTP:HN1	1.63	0.47
1:M:246:GLY:HA3	1:M:356:ASN:HA	1.96	0.47
2:N:282:GLN:O	2:P:60:LYS:HG3	2.15	0.47
2:B:177:VAL:CG2	1:I:329:ASN:HA	2.45	0.47
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.96	0.47
1:G:176:GLN:HB3	2:H:333:LEU:HD13	1.97	0.47
1:G:228:ASN:HD21	3:G:501:GTP:HN1	1.63	0.47
1:G:246:GLY:HA3	1:G:356:ASN:HA	1.96	0.47
2:L:345:GLU:H	2:L:345:GLU:CD	2.10	0.47
1:O:404:PHE:HA	2:P:260:VAL:O	2.14	0.47
1:Q:181:VAL:N	2:R:352:LYS:CD	2.78	0.47
1:Q:332:ILE:HA	1:Q:335:ILE:HG12	1.97	0.47
2:B:176:LYS:HD3	1:I:333:ALA:CB	2.42	0.46
1:C:325:PRO:HG2	2:N:224:TYR:CE1	2.50	0.46
2:D:401:ARG:NH2	1:G:435:VAL:HG22	2.30	0.46
1:E:53:PHE:HB3	1:E:61:HIS:HB3	1.96	0.46
1:E:332:ILE:HA	1:E:335:ILE:HG12	1.97	0.46
1:G:100:ALA:CB	2:H:254:LYS:HB2	2.44	0.46
1:K:181:VAL:CG2	2:L:352:LYS:HE2	2.44	0.46
1:O:177:VAL:HG21	2:P:329:ASP:CB	2.45	0.46
1:O:210:TYR:OH	2:P:326:LYS:HA	2.03	0.46
1:Q:53:PHE:HB3	1:Q:61:HIS:HB3	1.97	0.46
1:Q:210:TYR:CD2	2:R:326:LYS:CB	2.98	0.46
1:C:404:PHE:H	2:D:261:PRO:C	2.17	0.46
1:K:53:PHE:HB3	1:K:61:HIS:HB3	1.97	0.46
1:O:177:VAL:HG21	2:P:329:ASP:HB3	1.98	0.46
1:A:100:ALA:HA	2:B:254:LYS:HD2	1.96	0.46
2:B:282:GLN:O	2:F:60:LYS:HG3	2.15	0.46
2:B:332:MET:HA	2:B:332:MET:CE	2.46	0.46
2:B:407:TRP:CZ2	1:I:260:VAL:CB	2.87	0.46
2:B:407:TRP:CH2	1:I:256:GLN:CG	2.96	0.46
2:F:345:GLU:H	2:F:345:GLU:CD	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ALA:HB1	2:H:254:LYS:CA	2.44	0.46
1:G:181:VAL:HG23	2:H:352:LYS:CE	2.43	0.46
1:G:210:TYR:CD1	2:H:326:LYS:HD2	2.51	0.46
2:J:332:MET:HA	2:J:332:MET:CE	2.46	0.46
1:A:394:LYS:O	2:B:348:PRO:HG3	2.15	0.46
2:F:404:PHE:CE2	1:K:258:ASN:O	2.67	0.46
1:I:406:HIS:HE1	2:J:260:VAL:C	2.14	0.46
1:M:100:ALA:C	2:N:254:LYS:HG3	2.36	0.46
2:P:332:MET:HA	2:P:332:MET:CE	2.46	0.46
1:Q:96:LYS:O	2:R:2:ARG:NE	2.48	0.46
1:A:177:VAL:CG2	2:B:329:ASP:HB3	2.46	0.46
1:C:176:GLN:HG3	2:D:333:LEU:CD2	2.44	0.46
1:C:210:TYR:CE2	2:D:326:LYS:CB	2.98	0.46
1:C:332:ILE:HA	1:C:335:ILE:HG12	1.97	0.46
1:E:210:TYR:HB3	2:F:326:LYS:HE2	1.96	0.46
1:G:401:LYS:NZ	2:H:346:TRP:NE1	2.64	0.46
1:I:181:VAL:HG23	2:J:352:LYS:CE	2.43	0.46
1:Q:105:ARG:HH22	2:R:253:ARG:CZ	2.23	0.46
1:A:100:ALA:C	2:B:254:LYS:CD	2.83	0.46
1:A:181:VAL:HB	2:B:352:LYS:CG	2.45	0.46
1:A:348:PRO:CD	2:P:398:MET:SD	3.03	0.46
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.69	0.46
2:F:96:GLN:NE2	1:K:2:ARG:N	2.64	0.46
2:F:332:MET:HA	2:F:332:MET:CE	2.46	0.46
1:G:332:ILE:HA	1:G:335:ILE:HG12	1.97	0.46
2:H:288:VAL:HB	2:H:327:GLU:HG2	1.96	0.46
1:I:72:PRO:HB2	2:J:48:ARG:HH12	1.80	0.46
1:O:407:TRP:CD1	2:P:257:VAL:HA	2.50	0.46
2:R:332:MET:HA	2:R:332:MET:CE	2.46	0.46
1:A:210:TYR:HB3	2:B:326:LYS:HE2	1.96	0.46
1:A:404:PHE:CZ	2:B:314:THR:HG22	2.41	0.46
1:C:176:GLN:O	2:D:333:LEU:HD13	2.16	0.46
1:E:96:LYS:O	2:F:2:ARG:NE	2.49	0.46
1:E:210:TYR:CG	2:F:326:LYS:CD	2.99	0.46
1:E:348:PRO:CD	2:R:398:MET:SD	3.04	0.46
1:E:404:PHE:HA	2:F:261:PRO:HA	1.98	0.46
1:I:177:VAL:HG11	2:J:329:ASP:CG	2.35	0.46
1:M:332:ILE:HA	1:M:335:ILE:HG12	1.97	0.46
1:Q:404:PHE:HA	2:R:261:PRO:HA	1.95	0.46
1:A:100:ALA:HB1	2:B:254:LYS:CA	2.45	0.46
1:A:228:ASN:HD21	3:A:501:GTP:HN1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TRP:CD1	2:B:257:VAL:O	2.69	0.46
2:D:288:VAL:HB	2:D:327:GLU:HG2	1.96	0.46
1:E:177:VAL:HB	2:F:329:ASP:HB3	1.97	0.46
1:G:402:ARG:HD3	1:G:402:ARG:HA	1.69	0.46
1:I:100:ALA:C	2:J:254:LYS:CG	2.84	0.46
1:K:72:PRO:HB2	2:L:48:ARG:NH1	2.31	0.46
1:M:402:ARG:HD3	1:M:402:ARG:HA	1.69	0.46
2:N:288:VAL:HB	2:N:327:GLU:HG2	1.96	0.46
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.96	0.46
1:A:439:SER:OG	2:P:400:ARG:NH1	2.48	0.46
2:B:60:LYS:HG3	2:D:282:GLN:O	2.16	0.46
1:C:101:ASN:ND2	2:D:258:ASN:OD1	2.49	0.46
1:C:404:PHE:HE2	2:D:258:ASN:C	2.18	0.46
1:E:397:LEU:HD13	2:F:345:GLU:O	2.16	0.46
2:F:404:PHE:HE2	1:K:258:ASN:CA	2.29	0.46
1:K:228:ASN:HD21	3:K:501:GTP:HN1	1.62	0.46
2:L:332:MET:HA	2:L:332:MET:CE	2.46	0.46
1:O:228:ASN:HD21	3:O:501:GTP:HN1	1.63	0.46
1:O:246:GLY:HA3	1:O:356:ASN:HA	1.96	0.46
1:A:406:HIS:HE1	2:B:260:VAL:HG12	1.69	0.46
1:C:177:VAL:HG11	2:D:329:ASP:CG	2.36	0.46
1:I:101:ASN:CB	2:J:254:LYS:HG3	2.46	0.46
1:I:397:LEU:C	2:J:346:TRP:O	2.55	0.46
1:K:407:TRP:NE1	2:L:260:VAL:O	2.49	0.46
1:M:181:VAL:N	2:N:352:LYS:CD	2.79	0.46
1:M:224:TYR:CE2	2:N:325:MET:CG	2.89	0.46
1:O:181:VAL:HB	2:P:352:LYS:CE	2.45	0.46
1:Q:181:VAL:HB	2:R:352:LYS:CE	2.44	0.46
2:R:345:GLU:H	2:R:345:GLU:CD	2.10	0.46
1:A:176:GLN:O	2:B:333:LEU:HD13	2.16	0.45
1:C:101:ASN:CB	2:D:254:LYS:HG3	2.44	0.45
1:E:228:ASN:HD21	3:E:501:GTP:HN1	1.62	0.45
1:K:15:GLN:OE1	1:K:15:GLN:CA	2.61	0.45
1:K:406:HIS:HE1	2:L:260:VAL:C	2.15	0.45
1:M:407:TRP:CH2	2:N:256:ALA:HB1	2.51	0.45
1:Q:228:ASN:HD21	3:Q:501:GTP:HN1	1.63	0.45
1:A:100:ALA:CA	2:B:254:LYS:CB	2.84	0.45
1:A:190:THR:OG1	1:A:191:THR:N	2.49	0.45
1:G:401:LYS:HG2	2:H:346:TRP:CG	2.47	0.45
1:I:228:ASN:HD21	3:I:501:GTP:HN1	1.63	0.45
2:J:142:GLY:HA3	2:J:183:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:210:TYR:OH	2:P:326:LYS:CA	2.44	0.45
1:Q:397:LEU:HB3	2:R:346:TRP:HA	1.98	0.45
2:B:142:GLY:HA3	2:B:183:GLU:HG3	1.97	0.45
1:C:2:ARG:HD3	2:N:72:PRO:HD2	1.99	0.45
1:C:348:PRO:HG3	2:N:398:MET:CG	2.47	0.45
2:D:210:TYR:HE2	1:G:326:LYS:HB2	1.74	0.45
2:D:332:MET:HA	2:D:332:MET:CE	2.46	0.45
1:E:397:LEU:HB3	2:F:346:TRP:C	2.36	0.45
2:H:332:MET:HA	2:H:332:MET:CE	2.46	0.45
1:I:101:ASN:ND2	2:J:258:ASN:OD1	2.49	0.45
2:P:142:GLY:HA3	2:P:183:GLU:HG3	1.97	0.45
2:D:28:HIS:NE2	2:D:243:ARG:NH1	2.65	0.45
1:I:246:GLY:HA3	1:I:356:ASN:HA	1.97	0.45
1:I:407:TRP:CG	2:J:257:VAL:HA	2.50	0.45
1:K:179:THR:HA	2:L:353:THR:N	2.27	0.45
2:N:28:HIS:NE2	2:N:243:ARG:NH1	2.65	0.45
2:N:332:MET:HA	2:N:332:MET:CE	2.46	0.45
1:A:72:PRO:HB2	2:B:48:ARG:HH12	1.80	0.45
1:A:101:ASN:ND2	2:B:258:ASN:OD1	2.49	0.45
2:B:401:ARG:HB2	1:I:346:TRP:CB	2.28	0.45
1:C:329:ASN:HB2	2:N:177:VAL:HG21	1.98	0.45
1:E:407:TRP:CD1	2:F:257:VAL:O	2.70	0.45
1:I:332:ILE:HA	1:I:335:ILE:HG12	1.97	0.45
1:M:100:ALA:HA	2:N:254:LYS:CD	2.46	0.45
1:M:403:ALA:HB1	2:N:261:PRO:CB	2.45	0.45
1:O:190:THR:OG1	1:O:191:THR:N	2.49	0.45
1:O:332:ILE:HA	1:O:335:ILE:HG12	1.97	0.45
2:B:56:ALA:HB2	2:D:283:TYR:CA	2.44	0.45
2:B:167:ASN:C	2:B:167:ASN:OD1	2.55	0.45
2:B:400:ARG:NH1	1:I:439:SER:OG	2.48	0.45
1:C:210:TYR:CG	2:D:326:LYS:CD	2.99	0.45
2:D:142:GLY:HA3	2:D:183:GLU:HG3	1.97	0.45
1:E:15:GLN:OE1	1:E:15:GLN:CA	2.61	0.45
2:H:28:HIS:NE2	2:H:243:ARG:NH1	2.65	0.45
1:I:181:VAL:CG2	2:J:352:LYS:CE	2.94	0.45
1:I:398:MET:CG	2:J:348:PRO:HD2	2.43	0.45
1:I:407:TRP:CZ2	2:J:256:ALA:C	2.90	0.45
1:M:177:VAL:HG21	2:N:329:ASP:HB3	1.99	0.45
1:M:313:MET:SD	1:M:435:VAL:HG11	2.57	0.45
1:A:332:ILE:HA	1:A:335:ILE:HG12	1.97	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:398:MET:HG2	1:K:348:PRO:HD2	1.99	0.45
1:I:179:THR:HG21	2:J:353:THR:HG1	1.77	0.45
2:J:167:ASN:C	2:J:167:ASN:OD1	2.56	0.45
2:L:142:GLY:HA3	2:L:183:GLU:HG3	1.97	0.45
1:O:181:VAL:CG2	2:P:352:LYS:CE	2.95	0.45
1:Q:179:THR:HA	2:R:352:LYS:HA	1.97	0.45
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.50	0.45
1:A:260:VAL:HG12	2:P:406:HIS:NE2	2.30	0.45
2:B:28:HIS:NE2	2:B:243:ARG:NH1	2.65	0.45
1:C:181:VAL:HB	2:D:352:LYS:CG	2.47	0.45
1:C:260:VAL:O	2:N:406:HIS:NE2	2.45	0.45
2:D:167:ASN:C	2:D:167:ASN:OD1	2.56	0.45
2:F:142:GLY:HA3	2:F:183:GLU:HG3	1.97	0.45
2:F:167:ASN:OD1	2:F:167:ASN:C	2.56	0.45
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.50	0.45
1:K:398:MET:CG	2:L:348:PRO:HD2	2.43	0.45
2:L:167:ASN:OD1	2:L:167:ASN:C	2.56	0.45
1:M:255:PHE:HD1	1:M:255:PHE:HA	1.54	0.45
1:M:401:LYS:CD	2:N:346:TRP:CD2	2.93	0.45
2:N:142:GLY:HA3	2:N:183:GLU:HG3	1.97	0.45
2:R:167:ASN:OD1	2:R:167:ASN:C	2.56	0.45
2:R:331:GLN:HA	2:R:331:GLN:OE1	2.17	0.45
1:A:401:LYS:HG2	2:B:346:TRP:CD2	2.52	0.45
1:C:255:PHE:HD1	1:C:255:PHE:HA	1.54	0.45
1:E:348:PRO:CG	2:R:398:MET:CG	2.94	0.45
1:E:401:LYS:NZ	2:F:346:TRP:NE1	2.65	0.45
1:G:101:ASN:ND2	2:H:258:ASN:OD1	2.50	0.45
1:G:401:LYS:HZ3	2:H:346:TRP:HE1	1.65	0.45
2:H:167:ASN:C	2:H:167:ASN:OD1	2.56	0.45
2:N:167:ASN:C	2:N:167:ASN:OD1	2.56	0.45
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.50	0.45
2:P:167:ASN:C	2:P:167:ASN:OD1	2.56	0.45
2:R:142:GLY:HA3	2:R:183:GLU:HG3	1.97	0.45
1:A:313:MET:SD	1:A:435:VAL:HG11	2.57	0.45
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.80	0.45
1:C:348:PRO:HG3	2:N:398:MET:HG3	1.99	0.45
1:E:404:PHE:H	2:F:261:PRO:C	2.19	0.45
2:F:401:ARG:NH2	1:K:435:VAL:HG22	2.32	0.45
1:G:190:THR:OG1	1:G:191:THR:N	2.49	0.45
2:H:142:GLY:HA3	2:H:183:GLU:HG3	1.97	0.45
1:K:177:VAL:HG21	2:L:329:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:282:GLN:O	2:P:60:LYS:CG	2.65	0.45
2:P:28:HIS:NE2	2:P:243:ARG:NH1	2.65	0.45
1:Q:210:TYR:CE1	2:R:326:LYS:CA	2.76	0.45
1:A:177:VAL:HG11	2:B:329:ASP:CG	2.37	0.44
2:F:331:GLN:OE1	2:F:331:GLN:HA	2.17	0.44
1:G:313:MET:SD	1:G:435:VAL:HG11	2.57	0.44
2:L:139:HIS:O	2:L:170:SER:HA	2.16	0.44
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.17	0.44
1:M:101:ASN:CA	2:N:254:LYS:CD	2.95	0.44
2:N:139:HIS:O	2:N:170:SER:HA	2.16	0.44
1:O:210:TYR:CE1	2:P:326:LYS:CA	2.77	0.44
1:O:313:MET:SD	1:O:435:VAL:HG11	2.57	0.44
2:P:248:LEU:HD23	2:P:248:LEU:HA	1.80	0.44
1:Q:15:GLN:OE1	1:Q:15:GLN:CA	2.61	0.44
1:Q:313:MET:SD	1:Q:435:VAL:HG11	2.57	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.16	0.44
1:E:2:ARG:HG2	2:R:96:GLN:NE2	2.26	0.44
1:E:348:PRO:CD	2:R:398:MET:HG3	2.35	0.44
1:K:190:THR:OG1	1:K:191:THR:N	2.49	0.44
1:O:394:LYS:O	2:P:348:PRO:CG	2.64	0.44
1:C:407:TRP:CD1	2:D:257:VAL:O	2.70	0.44
1:E:313:MET:SD	1:E:435:VAL:HG11	2.57	0.44
2:F:139:HIS:O	2:F:170:SER:HA	2.16	0.44
1:I:313:MET:SD	1:I:435:VAL:HG11	2.57	0.44
1:K:179:THR:CB	2:L:353:THR:H	2.31	0.44
1:O:96:LYS:O	2:P:2:ARG:NE	2.50	0.44
1:A:181:VAL:HG11	2:B:258:ASN:O	2.17	0.44
1:A:397:LEU:HD13	2:B:345:GLU:O	2.18	0.44
1:A:404:PHE:CE2	2:B:258:ASN:C	2.88	0.44
1:C:96:LYS:O	2:D:2:ARG:NE	2.51	0.44
1:C:190:THR:OG1	1:C:191:THR:N	2.49	0.44
1:E:179:THR:HG21	2:F:248:LEU:CD1	2.48	0.44
1:E:190:THR:OG1	1:E:191:THR:N	2.49	0.44
1:E:210:TYR:CE2	2:F:326:LYS:CB	3.00	0.44
1:E:325:PRO:HG2	2:R:224:TYR:CE1	2.53	0.44
1:G:181:VAL:CG2	2:H:352:LYS:CE	2.94	0.44
1:K:313:MET:SD	1:K:435:VAL:HG11	2.57	0.44
1:A:96:LYS:O	2:B:2:ARG:NE	2.50	0.44
1:A:101:ASN:CB	2:B:254:LYS:CD	2.80	0.44
1:E:406:HIS:HE1	2:F:260:VAL:C	2.19	0.44
1:G:398:MET:CG	2:H:348:PRO:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:HIS:O	2:H:170:SER:HA	2.17	0.44
1:M:190:THR:OG1	1:M:191:THR:N	2.49	0.44
1:O:397:LEU:HB3	2:P:346:TRP:CA	2.47	0.44
2:P:331:GLN:OE1	2:P:331:GLN:HA	2.17	0.44
2:R:139:HIS:O	2:R:170:SER:HA	2.17	0.44
1:A:179:THR:HA	2:B:353:THR:N	2.26	0.44
1:C:439:SER:OG	2:N:400:ARG:NH1	2.48	0.44
2:F:28:HIS:NE2	2:F:243:ARG:NH1	2.65	0.44
2:L:28:HIS:NE2	2:L:243:ARG:NH1	2.65	0.44
1:M:221:ARG:N	1:M:222:PRO:CD	2.80	0.44
1:M:404:PHE:HA	2:N:260:VAL:O	2.18	0.44
1:M:407:TRP:CZ2	2:N:256:ALA:C	2.90	0.44
2:N:242:LEU:N	2:N:242:LEU:CD1	2.81	0.44
2:P:74:THR:OG1	2:P:75:MET:N	2.51	0.44
1:Q:398:MET:CG	2:R:348:PRO:HD2	2.45	0.44
2:R:28:HIS:NE2	2:R:243:ARG:NH1	2.65	0.44
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.17	0.44
1:C:221:ARG:N	1:C:222:PRO:CD	2.80	0.44
2:D:242:LEU:N	2:D:242:LEU:CD1	2.81	0.44
1:G:221:ARG:N	1:G:222:PRO:CD	2.80	0.44
1:G:255:PHE:HD1	1:G:255:PHE:HA	1.54	0.44
1:G:404:PHE:CE2	2:H:258:ASN:C	2.88	0.44
2:H:331:GLN:OE1	2:H:331:GLN:HA	2.17	0.44
2:J:283:TYR:CB	2:L:62:VAL:CG2	2.92	0.44
1:M:210:TYR:OH	2:N:326:LYS:HA	2.05	0.44
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.44
1:C:181:VAL:HA	2:D:352:LYS:HZ1	1.83	0.44
1:E:100:ALA:HA	2:F:254:LYS:CD	2.47	0.44
1:E:100:ALA:O	1:E:101:ASN:HB3	2.18	0.44
2:H:74:THR:OG1	2:H:75:MET:N	2.51	0.44
2:H:242:LEU:CD1	2:H:242:LEU:N	2.81	0.44
1:I:30:ILE:HG12	1:I:36:MET:SD	2.58	0.44
1:I:397:LEU:HD13	2:J:345:GLU:O	2.17	0.44
2:J:28:HIS:NE2	2:J:243:ARG:NH1	2.64	0.44
2:J:139:HIS:O	2:J:170:SER:HA	2.17	0.44
1:K:100:ALA:C	2:L:254:LYS:CG	2.86	0.44
1:K:210:TYR:CD2	2:L:326:LYS:CB	3.01	0.44
1:M:181:VAL:HB	2:N:352:LYS:CE	2.46	0.44
2:P:139:HIS:O	2:P:170:SER:HA	2.17	0.44
1:Q:190:THR:OG1	1:Q:191:THR:N	2.49	0.44
1:A:30:ILE:HG12	1:A:36:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:NE	2:B:253:ARG:HE	2.16	0.44
2:B:74:THR:OG1	2:B:75:MET:N	2.51	0.44
1:C:210:TYR:CE1	2:D:326:LYS:CA	2.93	0.44
1:C:407:TRP:NE1	2:D:260:VAL:O	2.51	0.44
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.17	0.44
1:E:97:GLU:HB3	2:F:253:ARG:HH22	1.82	0.44
1:G:100:ALA:O	1:G:101:ASN:HB3	2.18	0.44
1:I:284:GLU:N	1:K:56:THR:HG22	2.33	0.44
1:I:401:LYS:HG2	2:J:346:TRP:CG	2.46	0.44
1:K:221:ARG:N	1:K:222:PRO:CD	2.80	0.44
1:O:30:ILE:HG12	1:O:36:MET:SD	2.58	0.44
1:Q:100:ALA:O	1:Q:101:ASN:HB3	2.18	0.44
1:A:221:ARG:N	1:A:222:PRO:CD	2.80	0.43
2:D:177:VAL:CG2	1:G:329:ASN:HA	2.48	0.43
1:E:221:ARG:N	1:E:222:PRO:CD	2.80	0.43
1:I:190:THR:OG1	1:I:191:THR:N	2.49	0.43
1:I:221:ARG:N	1:I:222:PRO:CD	2.80	0.43
1:I:402:ARG:HD3	1:I:402:ARG:HA	1.69	0.43
2:J:74:THR:OG1	2:J:75:MET:N	2.51	0.43
2:J:248:LEU:HD23	2:J:248:LEU:HA	1.80	0.43
2:J:331:GLN:HA	2:J:331:GLN:OE1	2.17	0.43
2:L:242:LEU:N	2:L:242:LEU:CD1	2.81	0.43
1:M:177:VAL:HG21	2:N:329:ASP:CB	2.48	0.43
1:Q:221:ARG:N	1:Q:222:PRO:CD	2.80	0.43
2:D:74:THR:OG1	2:D:75:MET:N	2.51	0.43
2:D:407:TRP:CZ2	1:G:260:VAL:CB	2.92	0.43
2:D:407:TRP:CE2	1:G:260:VAL:HB	2.51	0.43
2:J:345:GLU:H	2:J:345:GLU:CD	2.10	0.43
1:K:100:ALA:O	1:K:101:ASN:HB3	2.18	0.43
1:K:181:VAL:CB	2:L:352:LYS:HE2	2.45	0.43
1:K:404:PHE:HA	2:L:261:PRO:HA	2.01	0.43
2:N:74:THR:OG1	2:N:75:MET:N	2.51	0.43
2:N:331:GLN:OE1	2:N:331:GLN:HA	2.17	0.43
1:O:177:VAL:CG1	2:P:329:ASP:OD1	2.67	0.43
1:O:284:GLU:N	1:Q:56:THR:HG22	2.33	0.43
1:O:401:LYS:CD	2:P:346:TRP:CD2	2.92	0.43
1:Q:105:ARG:HH22	2:R:253:ARG:NH2	2.02	0.43
1:Q:403:ALA:HB1	2:R:261:PRO:CB	2.48	0.43
2:R:242:LEU:N	2:R:242:LEU:CD1	2.81	0.43
1:A:403:ALA:HB1	2:B:261:PRO:HB3	1.99	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:LYS:CE	2:F:346:TRP:NE1	2.81	0.43
2:F:242:LEU:N	2:F:242:LEU:CD1	2.81	0.43
1:G:30:ILE:HG12	1:G:36:MET:SD	2.58	0.43
1:I:407:TRP:CD2	2:J:257:VAL:HG22	2.53	0.43
1:O:221:ARG:N	1:O:222:PRO:CD	2.80	0.43
1:A:179:THR:HG22	2:B:353:THR:CB	2.38	0.43
1:C:254:GLU:HB2	2:N:100:GLY:HA2	1.99	0.43
1:E:407:TRP:HB3	2:F:257:VAL:HG13	2.01	0.43
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.50	0.43
1:I:179:THR:CB	2:J:353:THR:H	2.32	0.43
1:O:407:TRP:CE2	2:P:256:ALA:O	2.69	0.43
2:P:61:TYR:CD1	2:P:61:TYR:N	2.86	0.43
1:Q:30:ILE:HG12	1:Q:36:MET:SD	2.58	0.43
1:Q:243:ARG:HA	1:Q:243:ARG:HE	1.81	0.43
2:B:398:MET:HG3	1:I:348:PRO:CD	2.38	0.43
2:B:407:TRP:CE2	1:I:256:GLN:O	2.72	0.43
1:C:210:TYR:HB3	2:D:326:LYS:HE2	1.99	0.43
1:E:30:ILE:HG12	1:E:36:MET:SD	2.58	0.43
2:F:183:GLU:N	2:F:184:PRO:CD	2.82	0.43
2:H:61:TYR:CD1	2:H:61:TYR:N	2.86	0.43
1:K:30:ILE:HG12	1:K:36:MET:SD	2.58	0.43
1:M:181:VAL:CG2	2:N:352:LYS:HE2	2.46	0.43
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.50	0.43
1:Q:72:PRO:HB2	2:R:48:ARG:HH12	1.82	0.43
1:Q:179:THR:HG21	2:R:353:THR:HG1	1.75	0.43
2:R:183:GLU:N	2:R:184:PRO:CD	2.82	0.43
2:D:404:PHE:CE2	1:G:258:ASN:CA	3.01	0.43
2:J:61:TYR:CD1	2:J:61:TYR:N	2.86	0.43
2:L:183:GLU:N	2:L:184:PRO:CD	2.82	0.43
1:M:30:ILE:HG12	1:M:36:MET:SD	2.58	0.43
2:N:61:TYR:CD1	2:N:61:TYR:N	2.86	0.43
1:O:404:PHE:HA	2:P:261:PRO:HA	1.98	0.43
1:Q:407:TRP:NE1	2:R:260:VAL:O	2.51	0.43
2:B:61:TYR:CD1	2:B:61:TYR:N	2.86	0.43
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.50	0.43
2:D:61:TYR:CD1	2:D:61:TYR:N	2.86	0.43
1:E:72:PRO:HB2	2:F:48:ARG:NH1	2.34	0.43
1:E:210:TYR:CE1	2:F:326:LYS:CA	2.93	0.43
1:E:210:TYR:CG	2:F:326:LYS:CB	3.02	0.43
1:E:397:LEU:HB2	2:F:348:PRO:HD3	2.01	0.43
2:F:407:TRP:CH2	1:K:256:GLN:CG	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:TRP:CD2	2:H:257:VAL:HG22	2.54	0.43
1:I:435:VAL:O	1:I:435:VAL:HG12	2.18	0.43
1:M:72:PRO:CB	2:N:48:ARG:HH12	2.30	0.43
1:M:73:THR:HG23	2:N:245:PRO:HG3	2.01	0.43
1:M:105:ARG:HH22	2:N:253:ARG:CZ	2.23	0.43
1:O:306:ASP:HA	1:O:307:PRO:HD3	1.91	0.43
1:O:397:LEU:HB3	2:P:346:TRP:HA	2.01	0.43
1:A:346:TRP:CB	2:P:401:ARG:HB3	2.40	0.43
1:A:401:LYS:HZ3	2:B:346:TRP:HE1	1.65	0.43
2:B:345:GLU:H	2:B:345:GLU:CD	2.10	0.43
1:E:177:VAL:HG11	2:F:329:ASP:CG	2.39	0.43
1:I:181:VAL:CB	2:J:352:LYS:HE2	2.47	0.43
1:I:394:LYS:HA	2:J:348:PRO:CG	2.35	0.43
2:J:242:LEU:N	2:J:242:LEU:CD1	2.81	0.43
1:O:101:ASN:N	2:P:254:LYS:CE	2.79	0.43
1:O:177:VAL:HG11	2:P:329:ASP:CG	2.38	0.43
2:P:242:LEU:CD1	2:P:242:LEU:N	2.81	0.43
1:Q:397:LEU:HB3	2:R:346:TRP:CA	2.48	0.43
1:A:100:ALA:CB	2:B:254:LYS:HB2	2.49	0.43
2:B:242:LEU:N	2:B:242:LEU:CD1	2.81	0.43
1:G:179:THR:HA	2:H:353:THR:N	2.25	0.43
1:G:397:LEU:C	2:H:346:TRP:O	2.58	0.43
1:I:326:LYS:HB3	1:I:326:LYS:HE3	1.84	0.43
1:K:177:VAL:HG11	2:L:329:ASP:CG	2.39	0.43
2:P:183:GLU:N	2:P:184:PRO:CD	2.82	0.43
1:A:2:ARG:CA	2:P:96:GLN:NE2	2.82	0.43
2:B:183:GLU:N	2:B:184:PRO:CD	2.82	0.43
1:E:243:ARG:HA	1:E:243:ARG:HE	1.81	0.43
1:G:101:ASN:CB	2:H:254:LYS:HG3	2.49	0.43
2:H:109:THR:OG1	2:H:110:GLU:N	2.51	0.43
2:L:74:THR:OG1	2:L:75:MET:N	2.51	0.43
1:O:224:TYR:CE2	2:P:325:MET:CG	2.84	0.43
1:Q:402:ARG:HD3	1:Q:402:ARG:HA	1.69	0.43
1:A:100:ALA:O	1:A:101:ASN:HB3	2.18	0.42
1:C:100:ALA:CA	2:D:254:LYS:CB	2.86	0.42
1:C:100:ALA:HB1	2:D:254:LYS:CA	2.48	0.42
1:C:326:LYS:HB3	1:C:326:LYS:HE3	1.83	0.42
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.42
1:E:256:GLN:O	2:R:407:TRP:NE1	2.52	0.42
2:F:407:TRP:CE2	1:K:260:VAL:HB	2.51	0.42
1:G:179:THR:HG22	2:H:353:THR:CB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:THR:CG2	2:H:353:THR:HG1	2.15	0.42
1:K:147:SER:HB2	1:K:190:THR:HG21	2.01	0.42
2:L:61:TYR:CD1	2:L:61:TYR:N	2.86	0.42
2:N:109:THR:OG1	2:N:110:GLU:N	2.51	0.42
1:O:100:ALA:O	1:O:101:ASN:HB3	2.18	0.42
1:O:435:VAL:O	1:O:435:VAL:HG12	2.18	0.42
1:Q:147:SER:HB2	1:Q:190:THR:HG21	2.01	0.42
1:Q:407:TRP:CZ2	2:R:256:ALA:C	2.92	0.42
1:A:283:HIS:C	1:E:56:THR:HG22	2.39	0.42
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.91	0.42
1:A:394:LYS:C	2:B:348:PRO:HG3	2.40	0.42
1:A:435:VAL:O	1:A:435:VAL:HG12	2.18	0.42
1:E:147:SER:HB2	1:E:190:THR:HG21	2.01	0.42
1:E:333:ALA:CB	2:R:176:LYS:HD3	2.45	0.42
2:F:74:THR:OG1	2:F:75:MET:N	2.51	0.42
1:G:72:PRO:HB2	2:H:48:ARG:HH12	1.84	0.42
1:I:254:GLU:HA	1:I:257:THR:OG1	2.20	0.42
2:J:109:THR:OG1	2:J:110:GLU:N	2.51	0.42
1:K:177:VAL:CG2	2:L:329:ASP:HB3	2.49	0.42
1:K:404:PHE:CE2	2:L:258:ASN:C	2.92	0.42
1:M:326:LYS:HB3	1:M:326:LYS:HE3	1.83	0.42
1:O:254:GLU:HA	1:O:257:THR:OG1	2.20	0.42
1:O:401:LYS:HG2	2:P:346:TRP:HB3	1.98	0.42
2:R:61:TYR:CD1	2:R:61:TYR:N	2.86	0.42
1:A:254:GLU:HA	1:A:257:THR:OG1	2.20	0.42
2:B:109:THR:OG1	2:B:110:GLU:N	2.51	0.42
1:C:100:ALA:O	1:C:101:ASN:HB3	2.18	0.42
1:E:177:VAL:HG21	2:F:329:ASP:CB	2.50	0.42
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.69	0.42
1:G:254:GLU:HA	1:G:257:THR:OG1	2.20	0.42
1:G:326:LYS:HE3	1:G:326:LYS:HB3	1.84	0.42
2:J:183:GLU:N	2:J:184:PRO:CD	2.82	0.42
1:K:254:GLU:HA	1:K:257:THR:OG1	2.20	0.42
1:M:177:VAL:CG2	2:N:329:ASP:HB3	2.49	0.42
1:Q:407:TRP:CH2	2:R:256:ALA:HB1	2.54	0.42
2:R:109:THR:OG1	2:R:110:GLU:N	2.51	0.42
2:B:282:GLN:O	2:F:60:LYS:CG	2.68	0.42
2:B:398:MET:CG	1:I:348:PRO:CG	2.96	0.42
1:C:100:ALA:C	2:D:254:LYS:CD	2.85	0.42
1:C:254:GLU:HA	1:C:257:THR:OG1	2.20	0.42
1:C:406:HIS:HE1	2:D:260:VAL:C	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:TRP:HZ3	2:R:403:ALA:CB	1.89	0.42
2:F:61:TYR:CD1	2:F:61:TYR:N	2.86	0.42
1:G:100:ALA:C	2:H:254:LYS:CG	2.87	0.42
1:G:105:ARG:HH22	2:H:253:ARG:NH2	2.09	0.42
1:G:179:THR:HG21	2:H:353:THR:HG1	1.81	0.42
1:I:404:PHE:H	2:J:261:PRO:C	2.23	0.42
1:K:243:ARG:HA	1:K:243:ARG:HE	1.81	0.42
1:K:402:ARG:HD3	1:K:402:ARG:HA	1.70	0.42
2:L:109:THR:OG1	2:L:110:GLU:N	2.51	0.42
1:M:100:ALA:O	1:M:101:ASN:HB3	2.18	0.42
1:M:254:GLU:HA	1:M:257:THR:OG1	2.20	0.42
1:M:397:LEU:HB3	2:N:346:TRP:HA	2.01	0.42
2:P:156:LYS:HA	2:P:156:LYS:HD2	1.89	0.42
2:B:156:LYS:HA	2:B:156:LYS:HD2	1.89	0.42
1:E:254:GLU:HA	1:E:257:THR:OG1	2.20	0.42
1:E:260:VAL:CB	2:R:407:TRP:HZ2	2.27	0.42
2:F:109:THR:OG1	2:F:110:GLU:N	2.51	0.42
1:G:181:VAL:CB	2:H:352:LYS:HE2	2.47	0.42
1:I:100:ALA:O	1:I:101:ASN:HB3	2.18	0.42
1:K:181:VAL:N	2:L:352:LYS:CD	2.82	0.42
1:K:401:LYS:NZ	2:L:346:TRP:NE1	2.67	0.42
1:M:404:PHE:HA	2:N:261:PRO:HA	1.98	0.42
2:P:109:THR:OG1	2:P:110:GLU:N	2.51	0.42
2:P:345:GLU:H	2:P:345:GLU:CD	2.10	0.42
1:Q:181:VAL:CG2	2:R:352:LYS:HE2	2.47	0.42
1:Q:254:GLU:HA	1:Q:257:THR:OG1	2.20	0.42
1:Q:401:LYS:HZ3	2:R:346:TRP:HE1	1.68	0.42
1:A:348:PRO:CG	2:P:398:MET:HG3	2.47	0.42
1:A:407:TRP:CG	2:B:257:VAL:HA	2.54	0.42
2:B:404:PHE:CE2	1:I:258:ASN:CA	3.01	0.42
2:D:400:ARG:NH1	1:G:439:SER:OG	2.48	0.42
2:F:408:TYR:N	2:F:408:TYR:CD1	2.88	0.42
1:G:407:TRP:CZ2	2:H:256:ALA:C	2.92	0.42
1:G:407:TRP:NE1	2:H:260:VAL:O	2.53	0.42
1:M:394:LYS:HZ3	2:N:349:ASN:ND2	2.09	0.42
1:O:177:VAL:CB	2:P:329:ASP:CB	2.96	0.42
2:R:74:THR:OG1	2:R:75:MET:N	2.51	0.42
1:A:333:ALA:CB	2:P:176:LYS:HD3	2.46	0.42
1:A:346:TRP:O	2:P:398:MET:HA	2.20	0.42
1:C:397:LEU:HD13	2:D:345:GLU:O	2.18	0.42
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ARG:HD3	2:R:72:PRO:HD2	2.02	0.42
2:F:177:VAL:CG2	1:K:329:ASN:HA	2.49	0.42
1:G:177:VAL:CG1	2:H:329:ASP:OD1	2.68	0.42
1:G:397:LEU:HD13	2:H:345:GLU:O	2.20	0.42
2:H:283:TYR:CD2	2:J:62:VAL:CG2	2.82	0.42
1:I:181:VAL:N	2:J:352:LYS:CD	2.82	0.42
1:I:306:ASP:HA	1:I:307:PRO:HD3	1.91	0.42
1:K:177:VAL:HG21	2:L:329:ASP:CB	2.50	0.42
1:K:210:TYR:OH	2:L:326:LYS:CA	2.49	0.42
2:N:183:GLU:N	2:N:184:PRO:CD	2.82	0.42
2:N:248:LEU:HD23	2:N:248:LEU:HA	1.80	0.42
2:R:408:TYR:N	2:R:408:TYR:CD1	2.87	0.42
1:A:147:SER:HB2	1:A:190:THR:HG21	2.01	0.42
2:B:224:TYR:CE1	1:I:325:PRO:HG2	2.55	0.42
2:D:183:GLU:N	2:D:184:PRO:CD	2.82	0.42
2:D:408:TYR:N	2:D:408:TYR:CD1	2.87	0.42
2:F:407:TRP:CZ2	1:K:260:VAL:CB	2.91	0.42
1:G:358:GLU:HA	1:G:359:PRO:HD2	1.90	0.42
1:I:147:SER:HB2	1:I:190:THR:HG21	2.01	0.42
2:J:156:LYS:HA	2:J:156:LYS:HD2	1.89	0.42
1:O:243:ARG:HA	1:O:243:ARG:HE	1.81	0.42
1:O:404:PHE:CZ	2:P:258:ASN:O	2.65	0.42
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.50	0.42
1:A:284:GLU:N	1:E:56:THR:CG2	2.83	0.42
2:B:403:ALA:CB	1:I:346:TRP:HZ3	1.93	0.42
2:B:408:TYR:N	2:B:408:TYR:CD1	2.87	0.42
1:C:147:SER:HB2	1:C:190:THR:HG21	2.01	0.42
1:E:177:VAL:CG2	2:F:329:ASP:HB3	2.49	0.42
1:E:401:LYS:CG	2:F:346:TRP:CB	2.70	0.42
1:G:147:SER:HB2	1:G:190:THR:HG21	2.01	0.42
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.50	0.42
1:K:404:PHE:H	2:L:261:PRO:C	2.22	0.42
2:L:408:TYR:N	2:L:408:TYR:CD1	2.87	0.42
2:N:408:TYR:N	2:N:408:TYR:CD1	2.88	0.42
1:O:176:GLN:CD	2:P:333:LEU:HD21	2.38	0.42
2:P:408:TYR:N	2:P:408:TYR:CD1	2.88	0.42
1:A:258:ASN:OD1	2:P:180:THR:HG23	2.19	0.42
1:E:179:THR:CB	2:F:353:THR:H	2.33	0.42
1:E:211:ASP:HA	1:E:214:ARG:HG2	2.02	0.42
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.50	0.42
1:I:101:ASN:CB	2:J:254:LYS:CD	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:403:ALA:HB1	2:J:261:PRO:HB3	2.02	0.42
1:K:176:GLN:HG3	2:L:333:LEU:CD2	2.38	0.42
1:M:147:SER:HB2	1:M:190:THR:HG21	2.01	0.42
1:M:179:THR:HA	2:N:352:LYS:HA	2.00	0.42
1:O:147:SER:HB2	1:O:190:THR:HG21	2.01	0.42
1:Q:211:ASP:HA	1:Q:214:ARG:HG2	2.02	0.42
1:A:56:THR:HG22	1:C:284:GLU:N	2.35	0.41
2:H:183:GLU:N	2:H:184:PRO:CD	2.82	0.41
2:H:408:TYR:N	2:H:408:TYR:CD1	2.87	0.41
1:K:147:SER:HB2	1:K:190:THR:CG2	2.50	0.41
1:K:181:VAL:CG2	2:L:352:LYS:CE	2.98	0.41
1:K:358:GLU:HA	1:K:359:PRO:HD2	1.90	0.41
1:Q:147:SER:HB2	1:Q:190:THR:CG2	2.50	0.41
1:A:176:GLN:HG3	2:B:333:LEU:CD2	2.43	0.41
1:A:243:ARG:HA	1:A:243:ARG:HE	1.81	0.41
1:A:248:LEU:HD21	5:P:901:GDP:C8	2.54	0.41
1:A:326:LYS:CG	2:P:210:TYR:CD2	3.03	0.41
1:C:358:GLU:HA	1:C:359:PRO:HD2	1.90	0.41
1:E:100:ALA:HB1	2:F:254:LYS:CA	2.47	0.41
1:E:394:LYS:C	2:F:348:PRO:HG3	2.40	0.41
1:G:407:TRP:CG	2:H:257:VAL:HA	2.54	0.41
2:J:103:TRP:CD1	2:J:103:TRP:C	2.94	0.41
2:J:408:TYR:N	2:J:408:TYR:CD1	2.88	0.41
1:K:211:ASP:HA	1:K:214:ARG:HG2	2.02	0.41
1:O:211:ASP:HA	1:O:214:ARG:HG2	2.02	0.41
1:Q:210:TYR:OH	2:R:326:LYS:CA	2.46	0.41
1:A:211:ASP:HA	1:A:214:ARG:HG2	2.02	0.41
2:B:103:TRP:CD1	2:B:103:TRP:C	2.94	0.41
1:E:147:SER:HB2	1:E:190:THR:CG2	2.51	0.41
1:E:254:GLU:HB2	2:R:100:GLY:HA2	2.01	0.41
1:E:260:VAL:HG12	2:R:406:HIS:NE2	2.35	0.41
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.80	0.41
1:I:211:ASP:HA	1:I:214:ARG:HG2	2.02	0.41
2:P:103:TRP:CD1	2:P:103:TRP:C	2.94	0.41
1:A:147:SER:HB2	1:A:190:THR:CG2	2.50	0.41
1:C:147:SER:HB2	1:C:190:THR:CG2	2.50	0.41
1:C:211:ASP:HA	1:C:214:ARG:HG2	2.02	0.41
1:E:181:VAL:HB	2:F:352:LYS:CG	2.48	0.41
1:G:211:ASP:HA	1:G:214:ARG:HG2	2.02	0.41
1:I:147:SER:HB2	1:I:190:THR:CG2	2.50	0.41
1:K:181:VAL:HA	2:L:352:LYS:HZ1	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:345:ASP:OD2	1:K:439:SER:OG	2.35	0.41
1:K:401:LYS:CE	2:L:346:TRP:NE1	2.83	0.41
1:M:211:ASP:HA	1:M:214:ARG:HG2	2.02	0.41
1:O:147:SER:HB2	1:O:190:THR:CG2	2.50	0.41
1:C:333:ALA:CB	2:N:176:LYS:HD3	2.47	0.41
1:C:348:PRO:CD	2:N:398:MET:SD	3.07	0.41
1:C:401:LYS:CG	2:D:346:TRP:CB	2.72	0.41
1:C:404:PHE:CE2	2:D:258:ASN:C	2.92	0.41
2:D:103:TRP:CD1	2:D:103:TRP:C	2.94	0.41
1:E:358:GLU:HA	1:E:359:PRO:HD2	1.90	0.41
1:G:147:SER:HB2	1:G:190:THR:CG2	2.50	0.41
1:G:297:GLU:HA	1:G:298:PRO:HD3	1.89	0.41
1:I:243:ARG:HA	1:I:243:ARG:HE	1.81	0.41
1:K:407:TRP:CZ2	2:L:256:ALA:C	2.94	0.41
2:N:103:TRP:CD1	2:N:103:TRP:C	2.94	0.41
1:O:388:TRP:CE3	1:O:388:TRP:CA	3.04	0.41
1:O:404:PHE:HD2	2:P:257:VAL:O	2.04	0.41
2:P:88:ARG:HA	2:P:89:PRO:HD3	1.86	0.41
1:A:388:TRP:CE3	1:A:388:TRP:CA	3.04	0.41
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.86	0.41
1:C:394:LYS:C	2:D:348:PRO:HG3	2.40	0.41
1:E:181:VAL:HA	2:F:352:LYS:HZ1	1.82	0.41
1:E:345:ASP:OD2	1:E:439:SER:OG	2.35	0.41
2:F:401:ARG:O	2:F:402:LYS:HB2	2.21	0.41
2:H:103:TRP:CD1	2:H:103:TRP:C	2.94	0.41
1:K:100:ALA:C	2:L:254:LYS:HG3	2.41	0.41
1:K:407:TRP:CG	2:L:257:VAL:HA	2.55	0.41
1:M:243:ARG:HA	1:M:243:ARG:HE	1.81	0.41
1:O:210:TYR:CE1	2:P:326:LYS:N	2.86	0.41
1:O:255:PHE:HD1	1:O:255:PHE:HA	1.54	0.41
2:R:401:ARG:O	2:R:402:LYS:HB2	2.21	0.41
1:C:388:TRP:CE3	1:C:388:TRP:CA	3.04	0.41
2:D:401:ARG:O	2:D:402:LYS:HB2	2.21	0.41
1:G:388:TRP:CE3	1:G:388:TRP:CA	3.04	0.41
2:L:401:ARG:O	2:L:402:LYS:HB2	2.21	0.41
1:M:147:SER:HB2	1:M:190:THR:CG2	2.50	0.41
1:M:388:TRP:CE3	1:M:388:TRP:CA	3.04	0.41
1:Q:388:TRP:CE3	1:Q:388:TRP:CA	3.04	0.41
1:A:255:PHE:HD1	1:A:255:PHE:HA	1.54	0.41
1:A:260:VAL:CG2	2:P:407:TRP:HZ2	2.34	0.41
1:A:329:ASN:HA	2:P:177:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLU:HA	1:C:298:PRO:HD3	1.89	0.41
1:E:346:TRP:CA	2:R:401:ARG:HG3	2.45	0.41
1:E:388:TRP:CE3	1:E:388:TRP:CA	3.04	0.41
1:K:100:ALA:CA	2:L:254:LYS:CB	2.82	0.41
1:M:297:GLU:HA	1:M:298:PRO:HD3	1.89	0.41
1:Q:100:ALA:HA	2:R:254:LYS:CG	2.51	0.41
1:A:101:ASN:ND2	2:B:258:ASN:HD21	2.16	0.41
1:A:350:GLY:O	2:P:181:VAL:CA	2.69	0.41
2:B:401:ARG:O	2:B:402:LYS:HB2	2.21	0.41
1:C:133:GLN:NE2	1:C:133:GLN:HA	2.36	0.41
1:C:181:VAL:HG11	2:D:258:ASN:O	2.20	0.41
2:D:398:MET:HG3	1:G:348:PRO:CD	2.42	0.41
2:D:400:ARG:NH2	1:G:345:ASP:OD1	2.50	0.41
1:G:133:GLN:NE2	1:G:133:GLN:HA	2.36	0.41
2:H:401:ARG:O	2:H:402:LYS:HB2	2.21	0.41
1:I:388:TRP:CE3	1:I:388:TRP:CA	3.04	0.41
1:K:388:TRP:CE3	1:K:388:TRP:CA	3.04	0.41
1:K:397:LEU:C	2:L:346:TRP:O	2.59	0.41
1:M:133:GLN:HA	1:M:133:GLN:NE2	2.36	0.41
1:M:358:GLU:HA	1:M:359:PRO:HD2	1.90	0.41
1:M:397:LEU:HB3	2:N:346:TRP:CA	2.49	0.41
1:M:404:PHE:CZ	2:N:258:ASN:O	2.71	0.41
2:N:401:ARG:O	2:N:402:LYS:HB2	2.21	0.41
1:O:283:HIS:C	1:Q:56:THR:HG22	2.41	0.41
1:O:401:LYS:HZ3	2:P:346:TRP:HE1	1.69	0.41
1:O:407:TRP:NE1	2:P:257:VAL:HA	2.31	0.41
2:P:401:ARG:O	2:P:402:LYS:HB2	2.21	0.41
1:Q:224:TYR:CE2	2:R:325:MET:CG	2.90	0.41
1:Q:404:PHE:HA	2:R:260:VAL:O	2.21	0.41
1:C:260:VAL:HG12	2:N:406:HIS:NE2	2.35	0.41
2:D:407:TRP:CE2	1:G:256:GLN:O	2.74	0.41
1:E:100:ALA:CA	2:F:254:LYS:CB	2.85	0.41
1:G:181:VAL:N	2:H:352:LYS:CD	2.84	0.41
1:I:181:VAL:HG11	2:J:258:ASN:O	2.20	0.41
1:I:398:MET:HG3	2:J:348:PRO:CD	2.47	0.41
2:J:401:ARG:O	2:J:402:LYS:HB2	2.21	0.41
1:O:90:GLU:OE2	1:O:121:ARG:NH1	2.54	0.41
1:A:90:GLU:OE2	1:A:121:ARG:NH1	2.55	0.40
1:C:243:ARG:HA	1:C:243:ARG:HE	1.81	0.40
1:E:133:GLN:NE2	1:E:133:GLN:HA	2.36	0.40
1:E:181:VAL:CG2	2:F:352:LYS:HE2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:TYR:CD1	2:F:202:TYR:N	2.90	0.40
1:I:90:GLU:OE2	1:I:121:ARG:NH1	2.54	0.40
1:I:133:GLN:NE2	1:I:133:GLN:HA	2.35	0.40
2:L:202:TYR:CD1	2:L:202:TYR:N	2.90	0.40
1:M:224:TYR:CG	2:N:325:MET:CG	2.87	0.40
1:O:133:GLN:NE2	1:O:133:GLN:HA	2.36	0.40
1:O:179:THR:HA	2:P:352:LYS:HA	2.03	0.40
1:O:394:LYS:HB3	2:P:348:PRO:HG2	2.03	0.40
1:Q:324:VAL:HA	1:Q:325:PRO:HD3	1.87	0.40
2:R:202:TYR:CD1	2:R:202:TYR:N	2.89	0.40
1:A:133:GLN:NE2	1:A:133:GLN:HA	2.36	0.40
1:A:179:THR:CB	2:B:353:THR:H	2.34	0.40
1:E:397:LEU:CB	2:F:346:TRP:O	2.62	0.40
1:E:401:LYS:HG2	2:F:346:TRP:CE3	2.55	0.40
2:H:347:ILE:HA	2:H:348:PRO:HD2	1.95	0.40
1:I:255:PHE:HD1	1:I:255:PHE:HA	1.54	0.40
1:K:133:GLN:NE2	1:K:133:GLN:HA	2.36	0.40
2:N:283:TYR:HD2	2:P:62:VAL:CG2	2.11	0.40
1:O:407:TRP:CD2	2:P:257:VAL:HG22	2.56	0.40
1:Q:133:GLN:HA	1:Q:133:GLN:NE2	2.36	0.40
1:Q:358:GLU:HA	1:Q:359:PRO:HD2	1.90	0.40
1:A:2:ARG:CB	2:P:96:GLN:NE2	2.82	0.40
1:A:104:ALA:HB1	1:A:411:GLU:HB2	2.04	0.40
1:A:394:LYS:CB	2:B:348:PRO:HG3	2.50	0.40
1:A:407:TRP:HB3	2:B:257:VAL:HG13	2.02	0.40
2:B:202:TYR:CD1	2:B:202:TYR:N	2.89	0.40
1:C:104:ALA:HB1	1:C:411:GLU:HB2	2.04	0.40
1:C:105:ARG:NE	2:D:253:ARG:HE	2.19	0.40
2:D:347:ILE:HA	2:D:348:PRO:HD2	1.95	0.40
1:E:101:ASN:CB	2:F:254:LYS:HG3	2.49	0.40
1:E:260:VAL:CG2	2:R:407:TRP:HZ2	2.35	0.40
1:G:179:THR:CB	2:H:353:THR:H	2.34	0.40
1:G:347:CYS:HA	1:G:348:PRO:HD2	1.87	0.40
1:I:63:PRO:O	1:I:91:GLN:NE2	2.50	0.40
1:I:100:ALA:C	2:J:254:LYS:HG3	2.42	0.40
1:I:104:ALA:HB1	1:I:411:GLU:HB2	2.04	0.40
1:O:181:VAL:CB	2:P:352:LYS:HE2	2.47	0.40
2:P:202:TYR:CD1	2:P:202:TYR:N	2.89	0.40
2:P:283:TYR:CD2	2:R:62:VAL:CG2	2.84	0.40
1:Q:104:ALA:HB1	1:Q:411:GLU:HB2	2.04	0.40
1:A:100:ALA:C	2:B:254:LYS:CG	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:THR:HA	2:F:352:LYS:HA	2.03	0.40
2:J:88:ARG:HA	2:J:89:PRO:HD3	1.86	0.40
2:J:202:TYR:CD1	2:J:202:TYR:N	2.90	0.40
1:K:90:GLU:OE2	1:K:121:ARG:NH1	2.54	0.40
1:K:398:MET:HG3	2:L:348:PRO:CD	2.46	0.40
1:M:101:ASN:CB	2:N:254:LYS:CG	2.90	0.40
1:M:104:ALA:HB1	1:M:411:GLU:HB2	2.04	0.40
1:O:104:ALA:HB1	1:O:411:GLU:HB2	2.04	0.40
1:Q:73:THR:HG23	2:R:245:PRO:HG3	2.04	0.40
1:A:63:PRO:O	1:A:91:GLN:NE2	2.50	0.40
1:A:276:ILE:HD13	1:A:276:ILE:HG21	1.91	0.40
1:E:104:ALA:HB1	1:E:411:GLU:HB2	2.04	0.40
1:E:404:PHE:HE2	2:F:258:ASN:C	2.25	0.40
1:G:104:ALA:HB1	1:G:411:GLU:HB2	2.04	0.40
2:J:388:PHE:N	2:J:388:PHE:CD1	2.89	0.40
1:K:104:ALA:HB1	1:K:411:GLU:HB2	2.04	0.40
2:L:283:TYR:CD1	2:L:283:TYR:N	2.90	0.40
1:O:63:PRO:O	1:O:91:GLN:NE2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	C	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	E	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	G	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	I	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	K	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	O	424/438 (97%)	409 (96%)	13 (3%)	2 (0%)	29	69
1	Q	424/438 (97%)	408 (96%)	14 (3%)	2 (0%)	29	69
2	B	424/426 (100%)	407 (96%)	14 (3%)	3 (1%)	22	62
2	D	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	F	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	H	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	J	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	L	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	N	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	P	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
2	R	424/426 (100%)	408 (96%)	13 (3%)	3 (1%)	22	62
All	All	7632/7776 (98%)	7351 (96%)	236 (3%)	45 (1%)	29	66

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLY
2	D	98	GLY
2	F	98	GLY
2	H	98	GLY
2	J	98	GLY
2	L	98	GLY
2	N	98	GLY
2	P	98	GLY
2	R	98	GLY
1	A	345	ASP
1	C	345	ASP
1	E	345	ASP
1	Q	345	ASP
2	B	350	ASN
2	D	350	ASN
2	F	350	ASN
1	G	345	ASP
2	H	350	ASN
1	I	345	ASP
2	J	350	ASN
1	K	345	ASP

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Mol	Chain	Res	Type
2	L	350	ASN
1	M	345	ASP
2	N	350	ASN
1	O	345	ASP
2	P	350	ASN
2	R	350	ASN
1	I	349	THR
1	M	349	THR
1	O	349	THR
1	A	349	THR
1	C	349	THR
1	E	349	THR
1	G	349	THR
1	K	349	THR
1	Q	349	THR
2	B	221	THR
2	D	221	THR
2	F	221	THR
2	H	221	THR
2	J	221	THR
2	L	221	THR
2	N	221	THR
2	P	221	THR
2	R	221	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	360/367 (98%)	359 (100%)	1 (0%)	92 94
1	C	360/367 (98%)	359 (100%)	1 (0%)	92 94
1	E	360/367 (98%)	359 (100%)	1 (0%)	92 94
1	G	360/367 (98%)	359 (100%)	1 (0%)	92 94
1	I	360/367 (98%)	359 (100%)	1 (0%)	92 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	360/367 (98%)	359 (100%)	1 (0%)	92	94
1	M	360/367 (98%)	359 (100%)	1 (0%)	92	94
1	O	360/367 (98%)	359 (100%)	1 (0%)	92	94
1	Q	360/367 (98%)	359 (100%)	1 (0%)	92	94
2	B	367/367 (100%)	367 (100%)	0	100	100
2	D	367/367 (100%)	367 (100%)	0	100	100
2	F	367/367 (100%)	367 (100%)	0	100	100
2	H	367/367 (100%)	367 (100%)	0	100	100
2	J	367/367 (100%)	367 (100%)	0	100	100
2	L	367/367 (100%)	367 (100%)	0	100	100
2	N	367/367 (100%)	367 (100%)	0	100	100
2	P	367/367 (100%)	367 (100%)	0	100	100
2	R	367/367 (100%)	367 (100%)	0	100	100
All	All	6543/6606 (99%)	6534 (100%)	9 (0%)	93	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	PHE
1	C	255	PHE
1	E	255	PHE
1	G	255	PHE
1	I	255	PHE
1	K	255	PHE
1	M	255	PHE
1	O	255	PHE
1	Q	255	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	101	ASN
1	A	128	GLN
1	A	133	GLN
1	A	301	GLN

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Mol	Chain	Res	Type
1	A	406	HIS
2	B	8	GLN
2	B	96	GLN
2	B	228	ASN
2	B	249	ASN
2	B	336	GLN
2	B	349	ASN
2	B	406	HIS
1	C	61	HIS
1	C	101	ASN
1	C	133	GLN
1	C	301	GLN
1	C	406	HIS
2	D	8	GLN
2	D	96	GLN
2	D	228	ASN
2	D	249	ASN
2	D	336	GLN
2	D	349	ASN
2	D	406	HIS
1	E	61	HIS
1	E	101	ASN
1	E	128	GLN
1	E	133	GLN
1	E	301	GLN
2	F	8	GLN
2	F	96	GLN
2	F	228	ASN
2	F	249	ASN
2	F	336	GLN
2	F	349	ASN
2	F	406	HIS
1	G	61	HIS
1	G	101	ASN
1	G	133	GLN
1	G	301	GLN
1	G	406	HIS
2	H	8	GLN
2	H	11	GLN
2	H	96	GLN
2	H	228	ASN
2	H	249	ASN

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Mol	Chain	Res	Type
2	H	336	GLN
2	H	349	ASN
1	I	61	HIS
1	I	101	ASN
1	I	128	GLN
1	I	133	GLN
1	I	301	GLN
1	I	406	HIS
2	J	8	GLN
2	J	11	GLN
2	J	96	GLN
2	J	228	ASN
2	J	249	ASN
2	J	336	GLN
2	J	349	ASN
1	K	61	HIS
1	K	101	ASN
1	K	128	GLN
1	K	133	GLN
1	K	301	GLN
1	K	406	HIS
2	L	8	GLN
2	L	11	GLN
2	L	96	GLN
2	L	228	ASN
2	L	249	ASN
2	L	336	GLN
2	L	349	ASN
1	M	61	HIS
1	M	101	ASN
1	M	258	ASN
1	M	301	GLN
2	N	8	GLN
2	N	96	GLN
2	N	228	ASN
2	N	249	ASN
2	N	336	GLN
2	N	349	ASN
2	N	406	HIS
1	O	61	HIS
1	O	101	ASN
1	O	301	GLN

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Mol	Chain	Res	Type
2	P	8	GLN
2	P	96	GLN
2	P	228	ASN
2	P	249	ASN
2	P	336	GLN
2	P	349	ASN
2	P	406	HIS
1	Q	61	HIS
1	Q	101	ASN
1	Q	258	ASN
1	Q	301	GLN
2	R	8	GLN
2	R	96	GLN
2	R	228	ASN
2	R	249	ASN
2	R	336	GLN
2	R	349	ASN
2	R	406	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GTP	Q	501	4	26,34,34	1.32	4 (15%)	32,54,54	1.11	3 (9%)
5	GDP	N	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.93	9 (30%)
5	GDP	F	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.92	9 (30%)
5	GDP	P	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.94	9 (30%)
5	GDP	H	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.94	9 (30%)
3	GTP	A	501	4	26,34,34	1.30	4 (15%)	32,54,54	1.10	3 (9%)
3	GTP	I	501	4	26,34,34	1.31	4 (15%)	32,54,54	1.10	3 (9%)
5	GDP	L	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.93	10 (33%)
3	GTP	E	501	4	26,34,34	1.31	4 (15%)	32,54,54	1.11	3 (9%)
3	GTP	G	501	4	26,34,34	1.31	4 (15%)	32,54,54	1.10	3 (9%)
5	GDP	R	901	-	24,30,30	2.74	9 (37%)	30,47,47	2.93	9 (30%)
3	GTP	M	501	4	26,34,34	1.29	4 (15%)	32,54,54	1.10	3 (9%)
3	GTP	K	501	4	26,34,34	1.29	4 (15%)	32,54,54	1.11	3 (9%)
5	GDP	D	901	-	24,30,30	2.73	9 (37%)	30,47,47	2.94	9 (30%)
3	GTP	C	501	4	26,34,34	1.29	4 (15%)	32,54,54	1.10	3 (9%)
5	GDP	B	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.93	9 (30%)
5	GDP	J	901	-	24,30,30	2.72	9 (37%)	30,47,47	2.93	9 (30%)
3	GTP	O	501	4	26,34,34	1.30	4 (15%)	32,54,54	1.10	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	Q	501	4	-	3/18/38/38	0/3/3/3
5	GDP	N	901	-	-	4/12/32/32	0/3/3/3
5	GDP	F	901	-	-	4/12/32/32	0/3/3/3
5	GDP	P	901	-	-	4/12/32/32	0/3/3/3
5	GDP	H	901	-	-	4/12/32/32	0/3/3/3
3	GTP	A	501	4	-	3/18/38/38	0/3/3/3
3	GTP	I	501	4	-	3/18/38/38	0/3/3/3
5	GDP	L	901	-	-	4/12/32/32	0/3/3/3
3	GTP	E	501	4	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	G	501	4	-	3/18/38/38	0/3/3/3
5	GDP	R	901	-	-	4/12/32/32	0/3/3/3
3	GTP	M	501	4	-	3/18/38/38	0/3/3/3
3	GTP	K	501	4	-	3/18/38/38	0/3/3/3
5	GDP	D	901	-	-	4/12/32/32	0/3/3/3
3	GTP	C	501	4	-	3/18/38/38	0/3/3/3
5	GDP	B	901	-	-	4/12/32/32	0/3/3/3
5	GDP	J	901	-	-	4/12/32/32	0/3/3/3
3	GTP	O	501	4	-	3/18/38/38	0/3/3/3

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	901	GDP	O4'-C1'	6.34	1.49	1.41
5	R	901	GDP	O4'-C1'	6.32	1.49	1.41
5	H	901	GDP	O4'-C1'	6.31	1.49	1.41
5	N	901	GDP	O4'-C1'	6.27	1.49	1.41
5	L	901	GDP	O4'-C1'	6.26	1.49	1.41
5	F	901	GDP	O4'-C1'	6.26	1.49	1.41
5	B	901	GDP	O4'-C1'	6.24	1.49	1.41
5	P	901	GDP	O4'-C1'	6.24	1.49	1.41
5	J	901	GDP	O4'-C1'	6.24	1.49	1.41
5	R	901	GDP	O6-C6	5.76	1.35	1.23
5	P	901	GDP	O6-C6	5.72	1.34	1.23
5	B	901	GDP	O6-C6	5.71	1.34	1.23
5	H	901	GDP	O6-C6	5.71	1.34	1.23
5	N	901	GDP	O6-C6	5.70	1.34	1.23
5	D	901	GDP	O6-C6	5.69	1.34	1.23
5	F	901	GDP	O6-C6	5.67	1.34	1.23
5	J	901	GDP	O6-C6	5.66	1.34	1.23
5	L	901	GDP	O6-C6	5.64	1.34	1.23
5	P	901	GDP	C2-N1	4.66	1.49	1.37
5	R	901	GDP	C2-N1	4.65	1.49	1.37
5	L	901	GDP	C2-N1	4.65	1.49	1.37
5	B	901	GDP	C2-N1	4.64	1.49	1.37
5	H	901	GDP	C2-N1	4.64	1.49	1.37
5	D	901	GDP	C2-N1	4.64	1.49	1.37
5	J	901	GDP	C2-N1	4.62	1.49	1.37
5	F	901	GDP	C2-N1	4.61	1.49	1.37
5	N	901	GDP	C2-N1	4.61	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	GDP	PB-O1B	4.17	1.64	1.50
5	J	901	GDP	PB-O1B	4.17	1.64	1.50
5	D	901	GDP	PB-O1B	4.16	1.64	1.50
5	L	901	GDP	PB-O1B	4.15	1.63	1.50
5	B	901	GDP	PB-O1B	4.14	1.63	1.50
5	H	901	GDP	PB-O1B	4.14	1.63	1.50
5	N	901	GDP	PB-O1B	4.13	1.63	1.50
5	P	901	GDP	PB-O1B	4.13	1.63	1.50
5	R	901	GDP	PB-O1B	4.12	1.63	1.50
5	L	901	GDP	PB-O2B	-3.80	1.40	1.54
5	N	901	GDP	PB-O2B	-3.80	1.40	1.54
5	H	901	GDP	PB-O2B	-3.80	1.40	1.54
5	D	901	GDP	PB-O2B	-3.79	1.40	1.54
5	P	901	GDP	PB-O2B	-3.79	1.40	1.54
5	J	901	GDP	PB-O2B	-3.77	1.40	1.54
5	R	901	GDP	PB-O2B	-3.77	1.40	1.54
5	B	901	GDP	PB-O2B	-3.77	1.40	1.54
5	F	901	GDP	PB-O2B	-3.77	1.40	1.54
3	I	501	GTP	C5-C6	-3.76	1.39	1.47
3	O	501	GTP	C5-C6	-3.76	1.39	1.47
3	G	501	GTP	C5-C6	-3.75	1.39	1.47
3	Q	501	GTP	C5-C6	-3.74	1.39	1.47
3	E	501	GTP	C5-C6	-3.72	1.39	1.47
3	K	501	GTP	C5-C6	-3.71	1.39	1.47
3	A	501	GTP	C5-C6	-3.71	1.39	1.47
3	C	501	GTP	C5-C6	-3.70	1.39	1.47
3	M	501	GTP	C5-C6	-3.69	1.39	1.47
5	F	901	GDP	C8-N7	3.69	1.41	1.35
5	J	901	GDP	C8-N7	3.63	1.41	1.35
5	L	901	GDP	C8-N7	3.63	1.41	1.35
5	R	901	GDP	C8-N7	3.62	1.41	1.35
5	B	901	GDP	C8-N7	3.60	1.41	1.35
5	P	901	GDP	C8-N7	3.60	1.41	1.35
5	N	901	GDP	C8-N7	3.57	1.41	1.35
5	D	901	GDP	C8-N7	3.57	1.41	1.35
5	H	901	GDP	C8-N7	3.56	1.41	1.35
5	R	901	GDP	C5-C6	-2.88	1.41	1.47
5	B	901	GDP	C5-C6	-2.86	1.41	1.47
5	P	901	GDP	C5-C6	-2.86	1.41	1.47
5	H	901	GDP	C5-C6	-2.85	1.41	1.47
5	D	901	GDP	C5-C6	-2.83	1.41	1.47
5	N	901	GDP	C5-C6	-2.83	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	GDP	C5-C6	-2.82	1.41	1.47
5	L	901	GDP	C5-C6	-2.82	1.41	1.47
5	J	901	GDP	C5-C6	-2.78	1.41	1.47
3	I	501	GTP	C6-N1	2.67	1.41	1.37
3	E	501	GTP	C6-N1	2.65	1.41	1.37
3	Q	501	GTP	C6-N1	2.64	1.41	1.37
3	A	501	GTP	C6-N1	2.64	1.41	1.37
3	C	501	GTP	C6-N1	2.62	1.41	1.37
3	G	501	GTP	C6-N1	2.62	1.41	1.37
3	M	501	GTP	C6-N1	2.55	1.41	1.37
3	O	501	GTP	C6-N1	2.55	1.41	1.37
3	K	501	GTP	C6-N1	2.53	1.41	1.37
3	Q	501	GTP	C8-N7	-2.45	1.30	1.35
3	A	501	GTP	C8-N7	-2.42	1.30	1.35
3	E	501	GTP	C8-N7	-2.41	1.30	1.35
5	D	901	GDP	C2-N3	-2.40	1.27	1.33
3	O	501	GTP	C8-N7	-2.39	1.30	1.35
3	G	501	GTP	C8-N7	-2.39	1.30	1.35
5	R	901	GDP	C2-N3	-2.39	1.27	1.33
3	C	501	GTP	C8-N7	-2.39	1.31	1.35
5	B	901	GDP	C2-N3	-2.37	1.27	1.33
5	L	901	GDP	C2-N3	-2.37	1.27	1.33
5	F	901	GDP	C2-N3	-2.36	1.27	1.33
5	N	901	GDP	C2-N3	-2.35	1.27	1.33
3	M	501	GTP	C8-N7	-2.35	1.31	1.35
3	Q	501	GTP	O4'-C1'	2.34	1.44	1.41
5	H	901	GDP	C2-N3	-2.34	1.27	1.33
5	J	901	GDP	C2-N3	-2.33	1.27	1.33
3	O	501	GTP	O4'-C1'	2.31	1.44	1.41
3	I	501	GTP	C8-N7	-2.31	1.31	1.35
5	P	901	GDP	C2-N3	-2.31	1.27	1.33
3	K	501	GTP	O4'-C1'	2.30	1.44	1.41
3	K	501	GTP	C8-N7	-2.29	1.31	1.35
3	I	501	GTP	O4'-C1'	2.28	1.44	1.41
3	M	501	GTP	O4'-C1'	2.27	1.44	1.41
3	E	501	GTP	O4'-C1'	2.27	1.44	1.41
3	G	501	GTP	O4'-C1'	2.25	1.44	1.41
3	A	501	GTP	O4'-C1'	2.22	1.44	1.41
3	C	501	GTP	O4'-C1'	2.21	1.44	1.41
5	D	901	GDP	O3'-C3'	2.16	1.48	1.43
5	F	901	GDP	O3'-C3'	2.12	1.48	1.43
5	B	901	GDP	O3'-C3'	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	901	GDP	O3'-C3'	2.11	1.47	1.43
5	N	901	GDP	O3'-C3'	2.10	1.47	1.43
5	H	901	GDP	O3'-C3'	2.09	1.47	1.43
5	P	901	GDP	O3'-C3'	2.09	1.47	1.43
5	L	901	GDP	O3'-C3'	2.09	1.47	1.43
5	R	901	GDP	O3'-C3'	2.06	1.47	1.43

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	901	GDP	C8-N7-C5	9.36	120.82	102.99
5	N	901	GDP	C8-N7-C5	9.35	120.80	102.99
5	B	901	GDP	C8-N7-C5	9.34	120.79	102.99
5	H	901	GDP	C8-N7-C5	9.34	120.79	102.99
5	P	901	GDP	C8-N7-C5	9.34	120.78	102.99
5	R	901	GDP	C8-N7-C5	9.34	120.78	102.99
5	J	901	GDP	C8-N7-C5	9.32	120.75	102.99
5	L	901	GDP	C8-N7-C5	9.32	120.74	102.99
5	F	901	GDP	C8-N7-C5	9.31	120.73	102.99
5	D	901	GDP	N2-C2-N3	6.27	131.95	119.74
5	R	901	GDP	N2-C2-N3	6.25	131.91	119.74
5	B	901	GDP	N2-C2-N3	6.24	131.88	119.74
5	L	901	GDP	N2-C2-N3	6.23	131.87	119.74
5	H	901	GDP	N2-C2-N3	6.23	131.87	119.74
5	N	901	GDP	N2-C2-N3	6.23	131.86	119.74
5	P	901	GDP	N2-C2-N3	6.22	131.84	119.74
5	F	901	GDP	N2-C2-N3	6.21	131.83	119.74
5	J	901	GDP	N2-C2-N3	6.21	131.82	119.74
5	P	901	GDP	C5-C6-N1	6.14	124.79	113.95
5	R	901	GDP	C5-C6-N1	6.12	124.76	113.95
5	H	901	GDP	C5-C6-N1	6.11	124.74	113.95
5	J	901	GDP	C5-C6-N1	6.10	124.73	113.95
5	B	901	GDP	C5-C6-N1	6.10	124.72	113.95
5	D	901	GDP	C5-C6-N1	6.08	124.68	113.95
5	N	901	GDP	C5-C6-N1	6.07	124.67	113.95
5	F	901	GDP	C5-C6-N1	6.07	124.67	113.95
5	L	901	GDP	C5-C6-N1	6.07	124.66	113.95
5	R	901	GDP	O6-C6-C5	-4.31	115.96	124.37
5	P	901	GDP	O6-C6-C5	-4.31	115.96	124.37
5	J	901	GDP	O6-C6-C5	-4.30	115.97	124.37
5	H	901	GDP	O6-C6-C5	-4.30	115.97	124.37
5	B	901	GDP	O6-C6-C5	-4.29	116.00	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	901	GDP	O6-C6-C5	-4.28	116.01	124.37
5	D	901	GDP	O6-C6-C5	-4.28	116.02	124.37
5	N	901	GDP	O6-C6-C5	-4.28	116.02	124.37
5	L	901	GDP	O6-C6-C5	-4.26	116.04	124.37
5	L	901	GDP	N2-C2-N1	-4.17	107.84	116.71
5	D	901	GDP	N2-C2-N1	-4.16	107.85	116.71
5	H	901	GDP	N2-C2-N1	-4.16	107.86	116.71
5	B	901	GDP	N2-C2-N1	-4.15	107.87	116.71
5	P	901	GDP	N2-C2-N1	-4.15	107.87	116.71
5	N	901	GDP	N2-C2-N1	-4.14	107.89	116.71
5	R	901	GDP	N2-C2-N1	-4.13	107.91	116.71
5	J	901	GDP	N2-C2-N1	-4.12	107.93	116.71
5	F	901	GDP	N2-C2-N1	-4.12	107.94	116.71
5	P	901	GDP	C2-N1-C6	-3.71	118.27	125.10
5	H	901	GDP	C2-N1-C6	-3.69	118.30	125.10
5	B	901	GDP	C2-N1-C6	-3.68	118.32	125.10
5	R	901	GDP	C2-N1-C6	-3.68	118.33	125.10
5	L	901	GDP	C2-N1-C6	-3.67	118.33	125.10
5	N	901	GDP	C2-N1-C6	-3.66	118.35	125.10
5	J	901	GDP	C2-N1-C6	-3.66	118.36	125.10
5	F	901	GDP	C2-N1-C6	-3.66	118.36	125.10
5	D	901	GDP	C2-N1-C6	-3.65	118.37	125.10
5	L	901	GDP	C2'-C3'-C4'	3.45	109.34	102.64
5	J	901	GDP	C2'-C3'-C4'	3.45	109.34	102.64
5	D	901	GDP	C2'-C3'-C4'	3.44	109.32	102.64
5	F	901	GDP	C2'-C3'-C4'	3.43	109.31	102.64
5	H	901	GDP	C2'-C3'-C4'	3.42	109.29	102.64
5	P	901	GDP	C2'-C3'-C4'	3.42	109.29	102.64
5	N	901	GDP	C2'-C3'-C4'	3.42	109.28	102.64
5	B	901	GDP	C2'-C3'-C4'	3.40	109.25	102.64
5	R	901	GDP	C2'-C3'-C4'	3.39	109.23	102.64
3	G	501	GTP	O2G-PG-O3B	2.66	113.57	104.64
3	Q	501	GTP	O2G-PG-O3B	2.66	113.57	104.64
3	E	501	GTP	O2G-PG-O3B	2.66	113.54	104.64
3	A	501	GTP	O2G-PG-O3B	2.65	113.53	104.64
3	M	501	GTP	O2G-PG-O3B	2.65	113.52	104.64
3	K	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
3	C	501	GTP	O2G-PG-O3B	2.64	113.49	104.64
3	O	501	GTP	O2G-PG-O3B	2.64	113.48	104.64
3	I	501	GTP	O2G-PG-O3B	2.63	113.45	104.64
5	N	901	GDP	O2'-C2'-C3'	2.31	119.30	111.82
5	H	901	GDP	O2'-C2'-C3'	2.31	119.30	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	901	GDP	O2'-C2'-C3'	2.31	119.29	111.82
5	P	901	GDP	O2'-C2'-C3'	2.30	119.27	111.82
5	D	901	GDP	O2'-C2'-C3'	2.30	119.26	111.82
5	J	901	GDP	O2'-C2'-C3'	2.29	119.23	111.82
5	B	901	GDP	O2'-C2'-C3'	2.29	119.23	111.82
5	R	901	GDP	O2'-C2'-C3'	2.29	119.23	111.82
5	L	901	GDP	O2'-C2'-C3'	2.29	119.22	111.82
5	D	901	GDP	O3B-PB-O2B	2.22	116.13	107.64
5	N	901	GDP	O3B-PB-O2B	2.22	116.13	107.64
5	J	901	GDP	O3B-PB-O2B	2.22	116.12	107.64
5	B	901	GDP	O3B-PB-O2B	2.22	116.11	107.64
5	L	901	GDP	O3B-PB-O2B	2.21	116.10	107.64
5	P	901	GDP	O3B-PB-O2B	2.21	116.09	107.64
5	F	901	GDP	O3B-PB-O2B	2.20	116.06	107.64
5	H	901	GDP	O3B-PB-O2B	2.20	116.05	107.64
5	R	901	GDP	O3B-PB-O2B	2.19	116.02	107.64
3	A	501	GTP	O5'-C5'-C4'	2.08	116.14	108.99
3	E	501	GTP	O5'-C5'-C4'	2.08	116.14	108.99
3	Q	501	GTP	O5'-C5'-C4'	2.08	116.14	108.99
3	G	501	GTP	O5'-C5'-C4'	2.07	116.13	108.99
3	I	501	GTP	O5'-C5'-C4'	2.06	116.10	108.99
3	O	501	GTP	O5'-C5'-C4'	2.06	116.09	108.99
3	M	501	GTP	O5'-C5'-C4'	2.06	116.07	108.99
3	C	501	GTP	O5'-C5'-C4'	2.06	116.07	108.99
3	K	501	GTP	O5'-C5'-C4'	2.05	116.06	108.99
3	I	501	GTP	O3G-PG-O3B	2.05	111.52	104.64
3	C	501	GTP	O3G-PG-O3B	2.05	111.50	104.64
3	M	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
3	E	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
3	G	501	GTP	O3G-PG-O3B	2.04	111.47	104.64
3	A	501	GTP	O3G-PG-O3B	2.04	111.46	104.64
3	K	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
3	Q	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
3	O	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
5	L	901	GDP	O4'-C4'-C3'	-2.01	101.14	105.11

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	GDP	PA-O3A-PB-O2B
5	B	901	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	D	901	GDP	PA-O3A-PB-O2B
5	D	901	GDP	C5'-O5'-PA-O3A
5	F	901	GDP	PA-O3A-PB-O2B
5	F	901	GDP	C5'-O5'-PA-O3A
5	H	901	GDP	PA-O3A-PB-O2B
5	H	901	GDP	C5'-O5'-PA-O3A
5	J	901	GDP	PA-O3A-PB-O2B
5	J	901	GDP	C5'-O5'-PA-O3A
5	L	901	GDP	PA-O3A-PB-O2B
5	L	901	GDP	C5'-O5'-PA-O3A
5	N	901	GDP	PA-O3A-PB-O2B
5	N	901	GDP	C5'-O5'-PA-O3A
5	P	901	GDP	PA-O3A-PB-O2B
5	P	901	GDP	C5'-O5'-PA-O3A
5	R	901	GDP	PA-O3A-PB-O2B
5	R	901	GDP	C5'-O5'-PA-O3A
3	A	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	Q	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	O4'-C4'-C5'-O5'
3	E	501	GTP	O4'-C4'-C5'-O5'
3	G	501	GTP	O4'-C4'-C5'-O5'
3	I	501	GTP	O4'-C4'-C5'-O5'
3	K	501	GTP	O4'-C4'-C5'-O5'
3	M	501	GTP	O4'-C4'-C5'-O5'
3	O	501	GTP	O4'-C4'-C5'-O5'
3	Q	501	GTP	O4'-C4'-C5'-O5'
5	B	901	GDP	C5'-O5'-PA-O2A
5	D	901	GDP	C5'-O5'-PA-O2A
5	F	901	GDP	C5'-O5'-PA-O2A
5	H	901	GDP	C5'-O5'-PA-O2A
5	J	901	GDP	C5'-O5'-PA-O2A
5	L	901	GDP	C5'-O5'-PA-O2A
5	N	901	GDP	C5'-O5'-PA-O2A
5	P	901	GDP	C5'-O5'-PA-O2A
5	R	901	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	501	GTP	O4'-C4'-C5'-O5'
5	B	901	GDP	PA-O3A-PB-O3B
5	D	901	GDP	PA-O3A-PB-O3B
5	F	901	GDP	PA-O3A-PB-O3B
5	H	901	GDP	PA-O3A-PB-O3B
5	J	901	GDP	PA-O3A-PB-O3B
5	L	901	GDP	PA-O3A-PB-O3B
5	N	901	GDP	PA-O3A-PB-O3B
5	P	901	GDP	PA-O3A-PB-O3B
5	R	901	GDP	PA-O3A-PB-O3B
3	A	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	C5'-O5'-PA-O1A
3	E	501	GTP	C5'-O5'-PA-O1A
3	G	501	GTP	C5'-O5'-PA-O1A
3	I	501	GTP	C5'-O5'-PA-O1A
3	K	501	GTP	C5'-O5'-PA-O1A
3	M	501	GTP	C5'-O5'-PA-O1A
3	O	501	GTP	C5'-O5'-PA-O1A
3	Q	501	GTP	C5'-O5'-PA-O1A

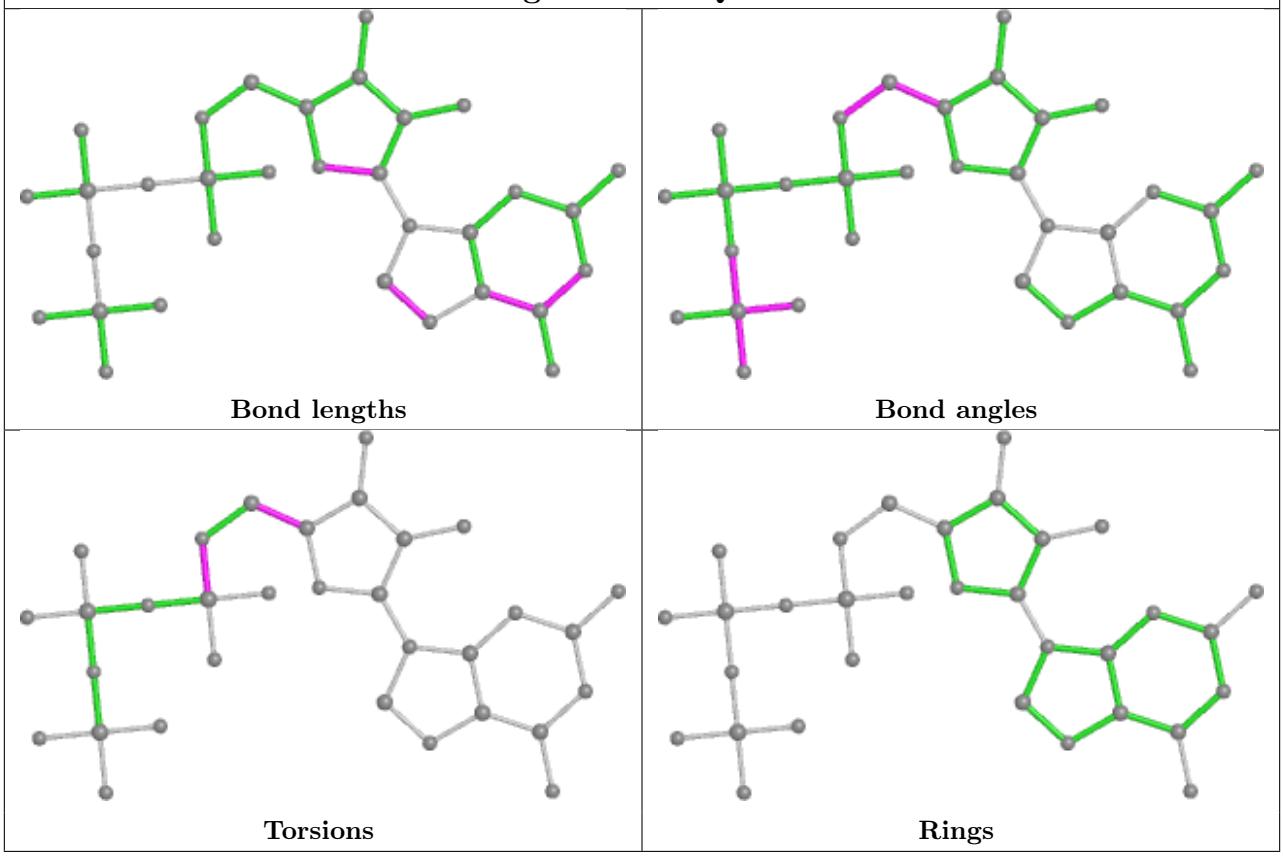
There are no ring outliers.

18 monomers are involved in 46 short contacts:

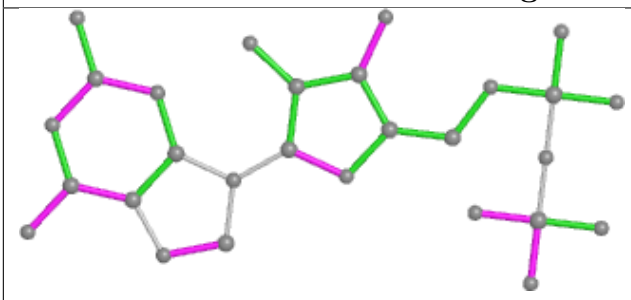
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	501	GTP	3	0
5	N	901	GDP	2	0
5	F	901	GDP	2	0
5	P	901	GDP	3	0
5	H	901	GDP	2	0
3	A	501	GTP	3	0
3	I	501	GTP	3	0
5	L	901	GDP	2	0
3	E	501	GTP	3	0
3	G	501	GTP	3	0
5	R	901	GDP	2	0
3	M	501	GTP	3	0
3	K	501	GTP	3	0
5	D	901	GDP	2	0
3	C	501	GTP	3	0
5	B	901	GDP	2	0
5	J	901	GDP	2	0
3	O	501	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

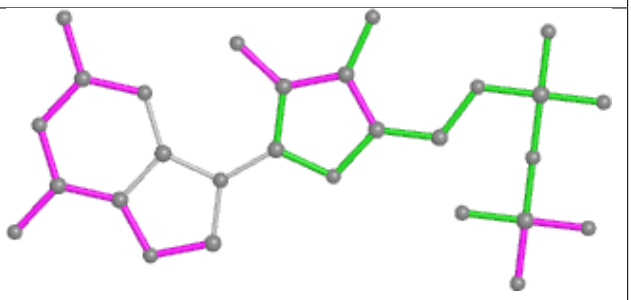
Ligand GTP Q 501



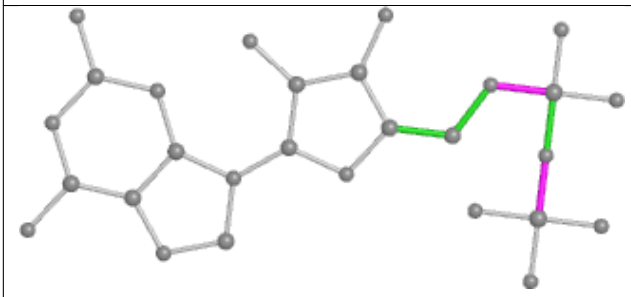
Ligand GDP N 901



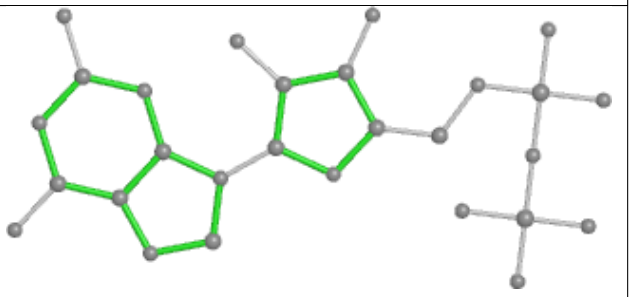
Bond lengths



Bond angles

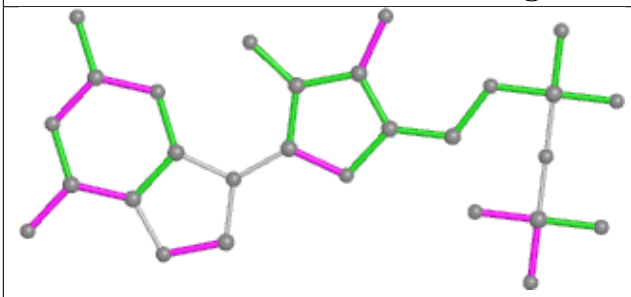


Torsions



Rings

Ligand GDP F 901



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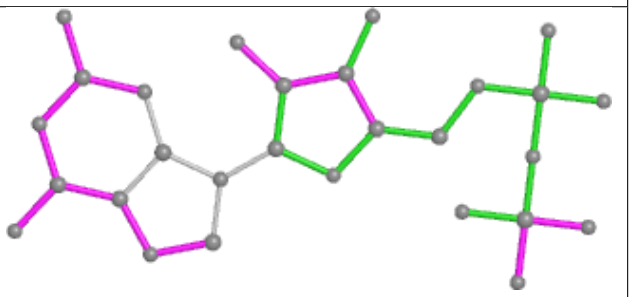

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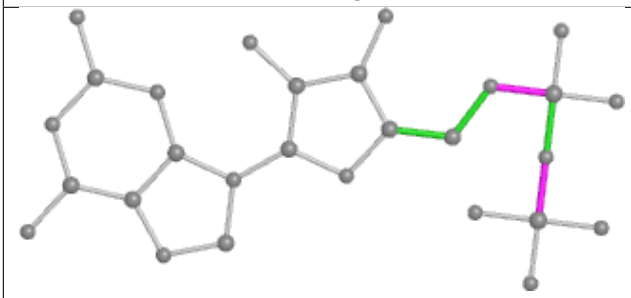
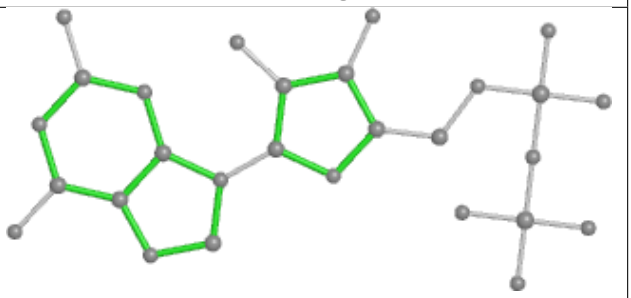
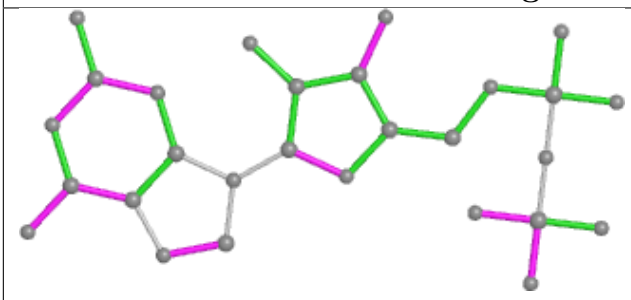


Torsions



Rings

Ligand GDP P 901



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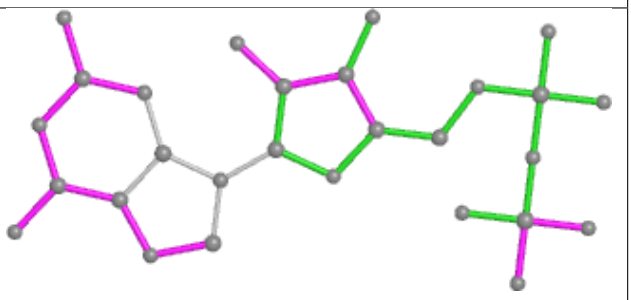

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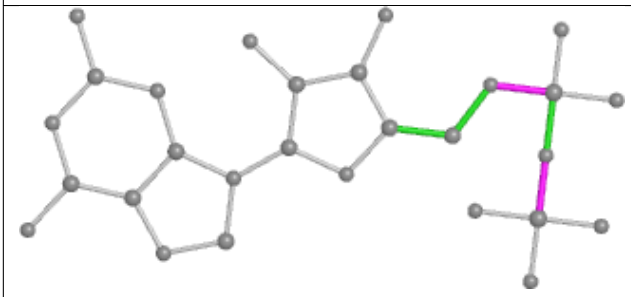

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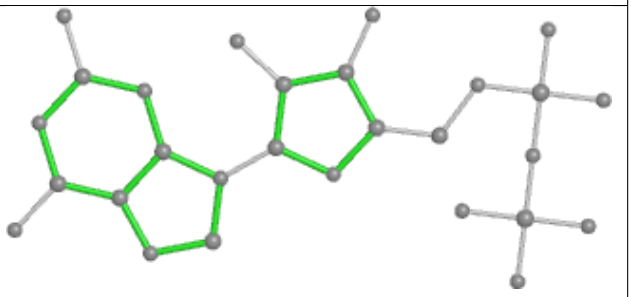
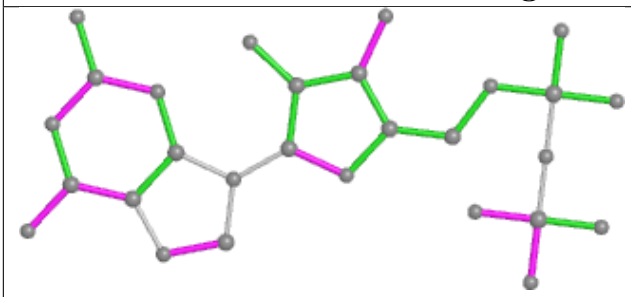


Rings

Ligand GDP H 901



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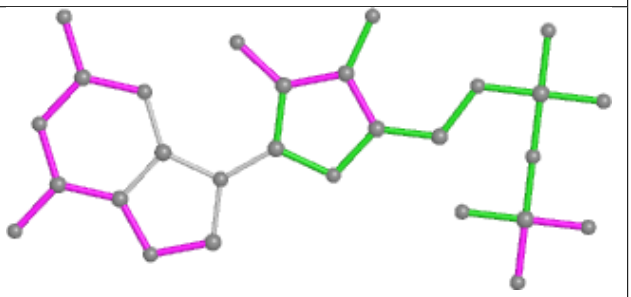

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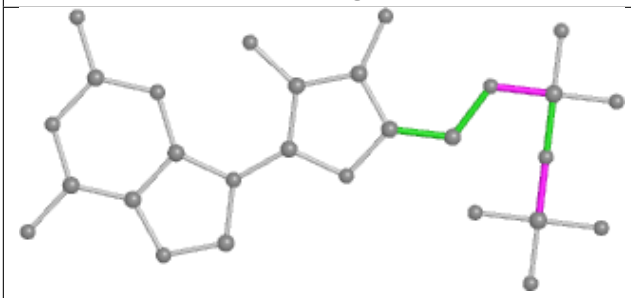

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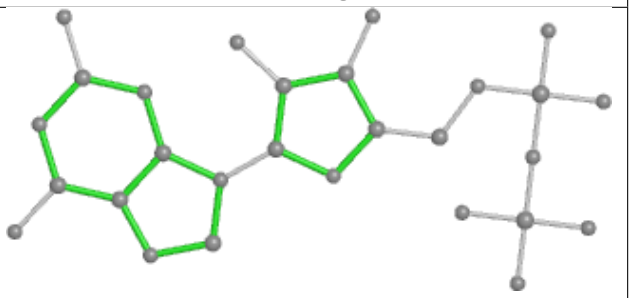
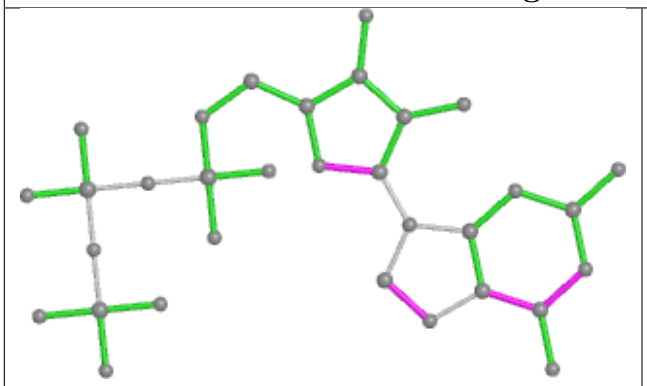


Rings

Ligand GTP A 501



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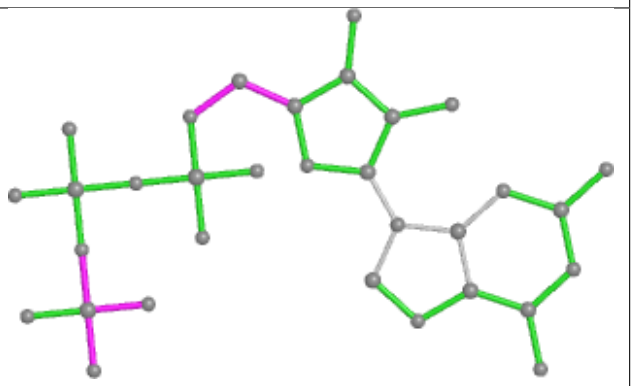

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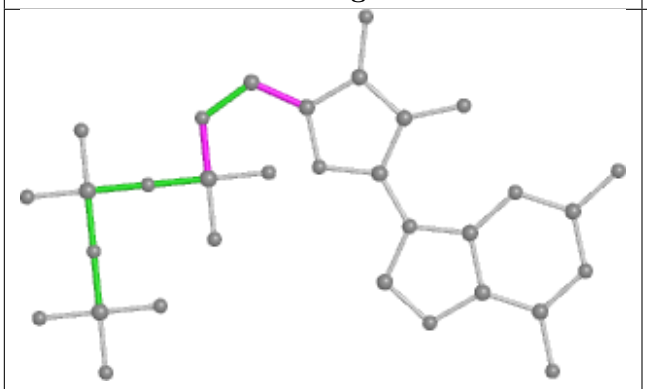

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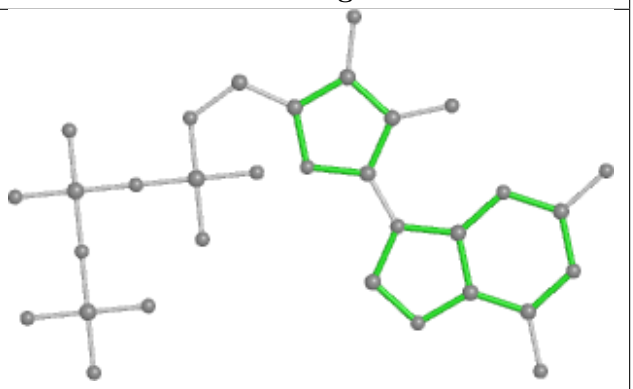
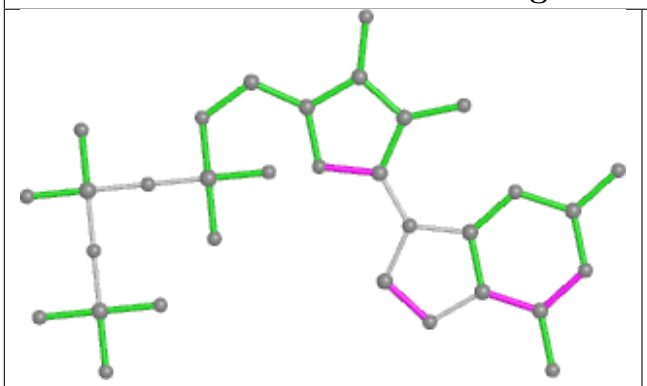


Rings

Ligand GTP I 501



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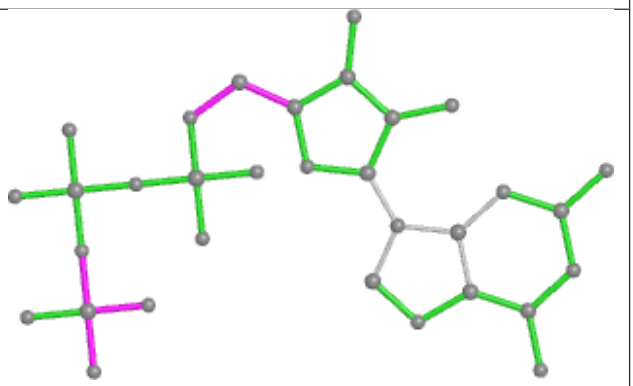

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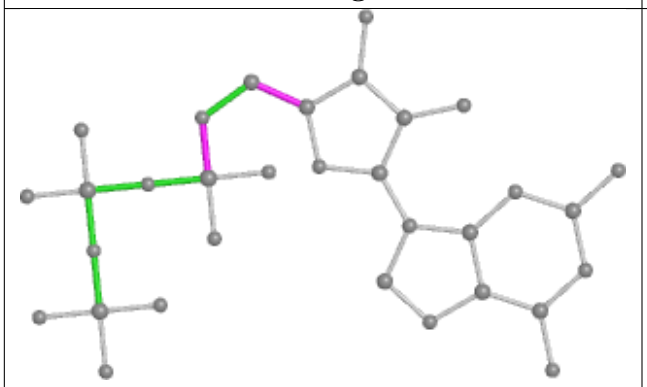

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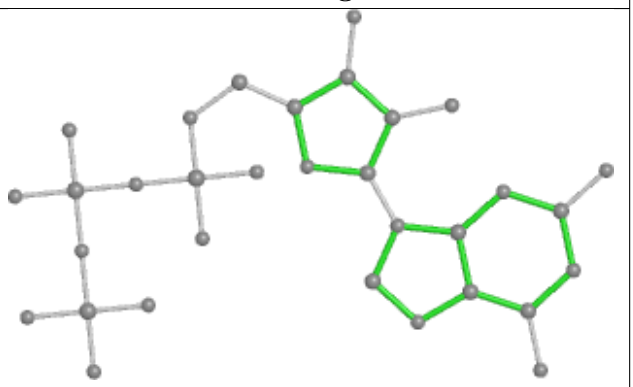
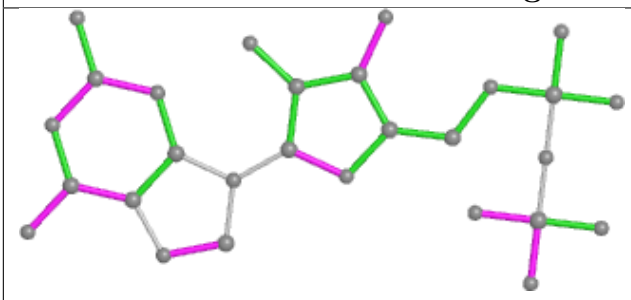


Rings

Ligand GDP L 901



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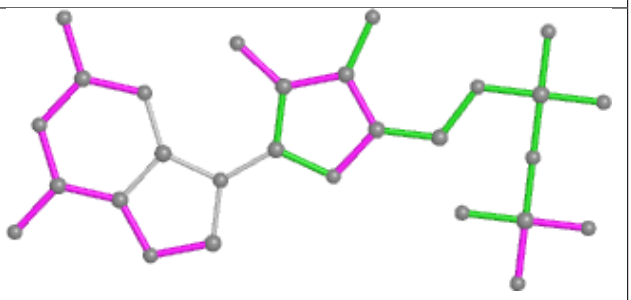

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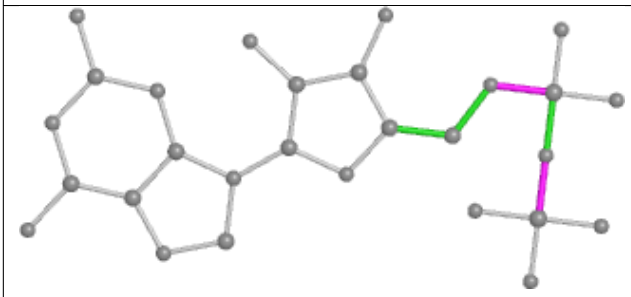

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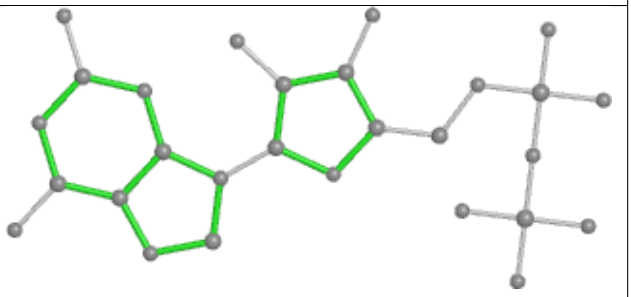
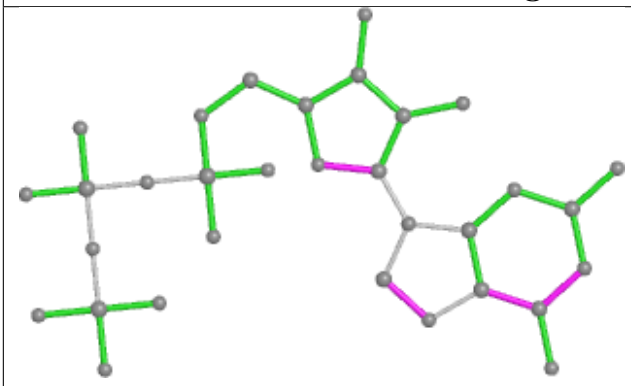


Rings

Ligand GTP E 501



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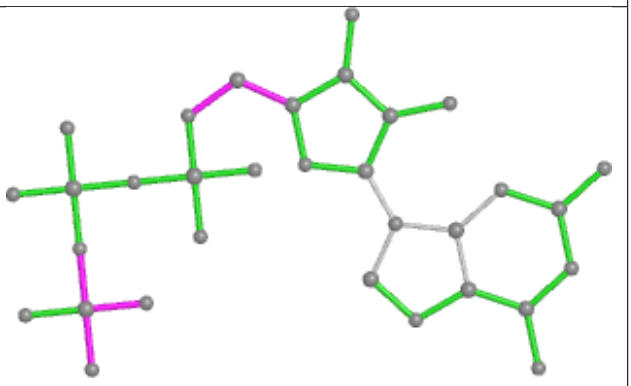

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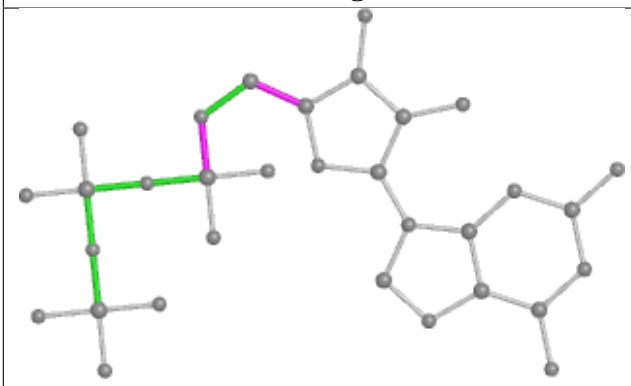

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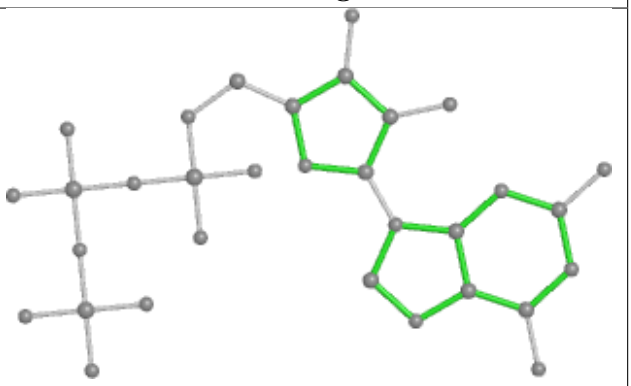

Rings

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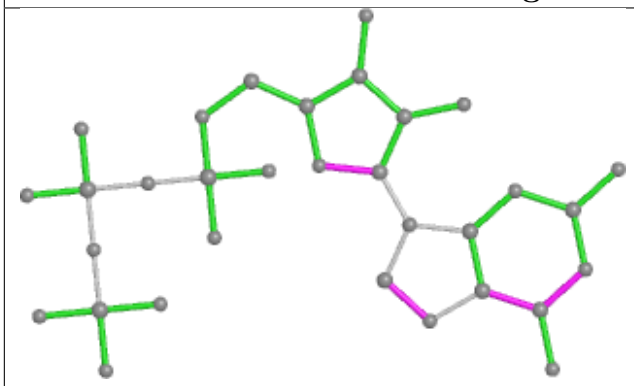

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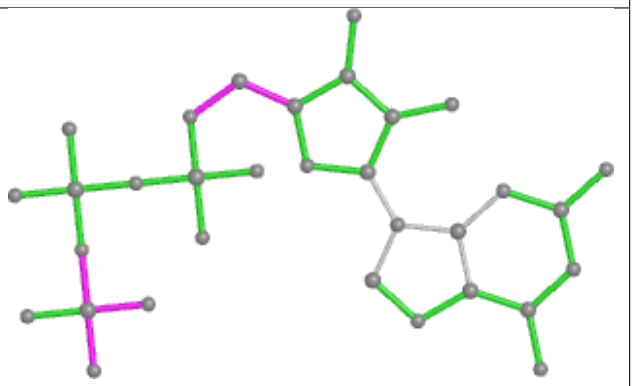

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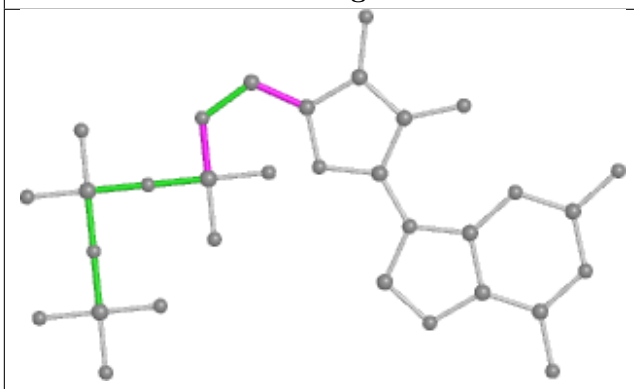

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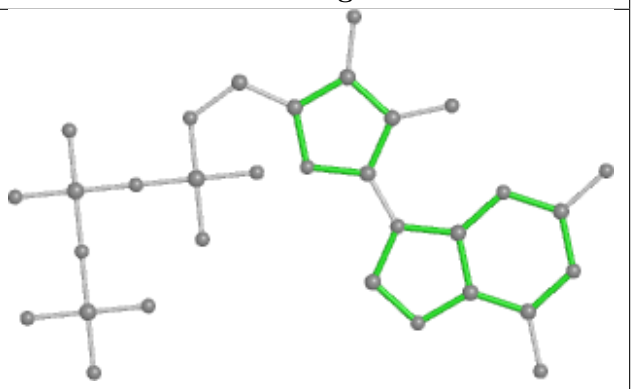
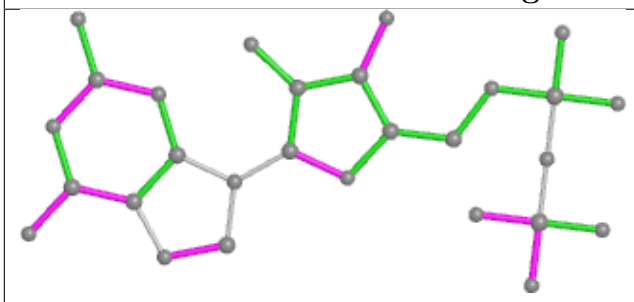


Rings

Ligand GDP R 901



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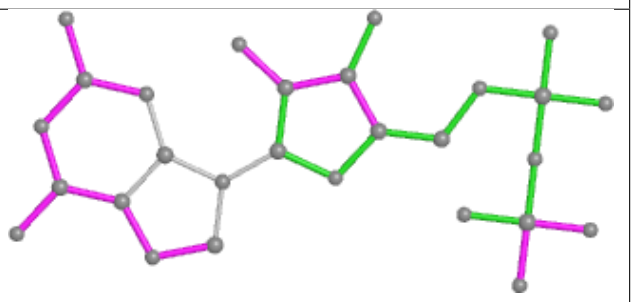

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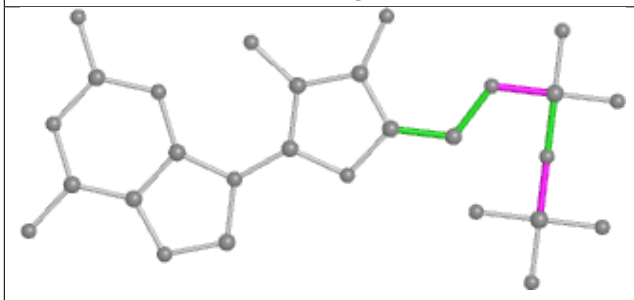

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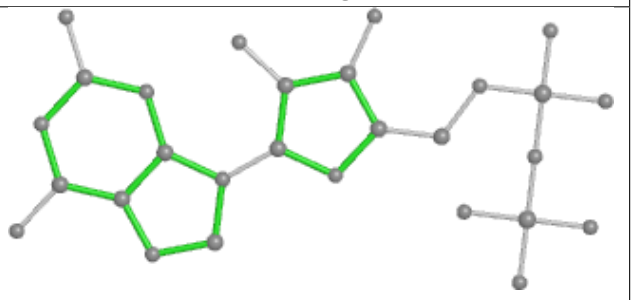
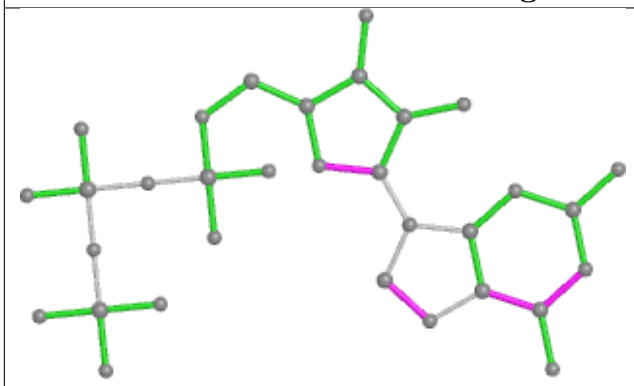


Rings

Ligand GTP M 501



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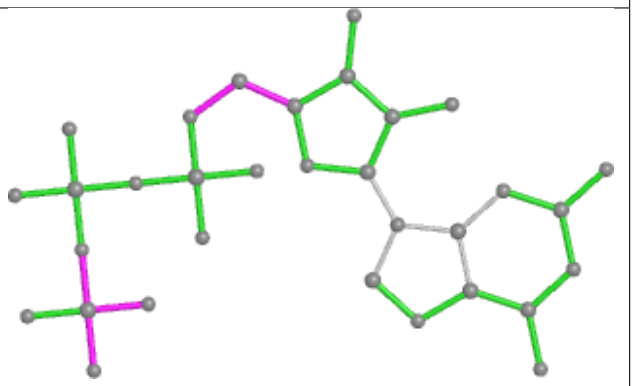

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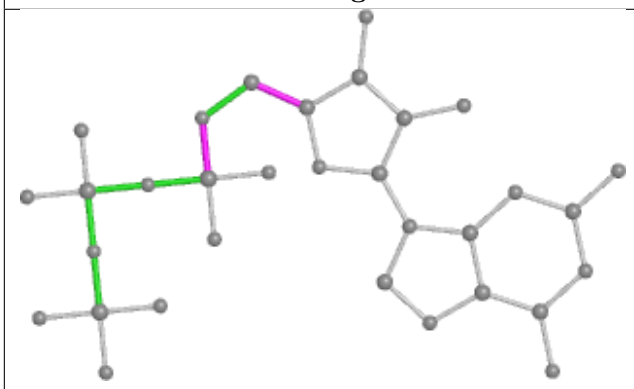

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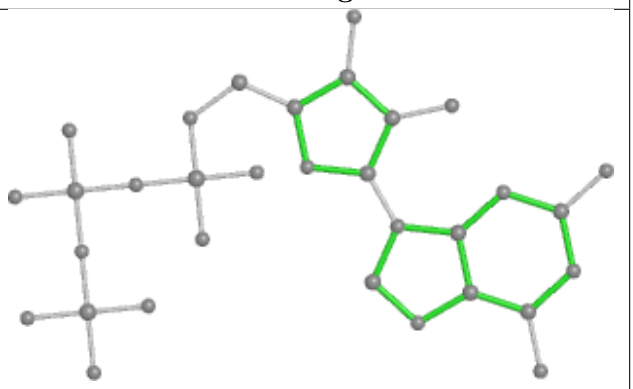
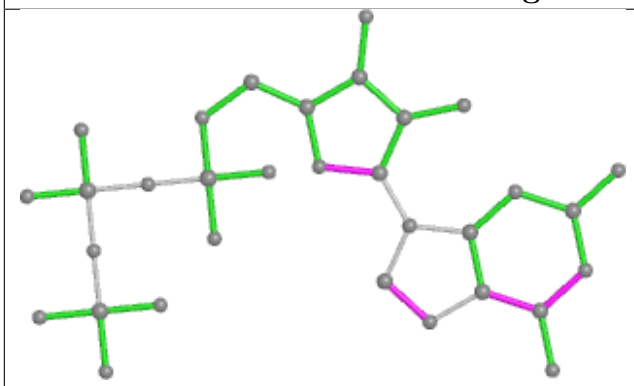


Rings

Ligand GTP K 501



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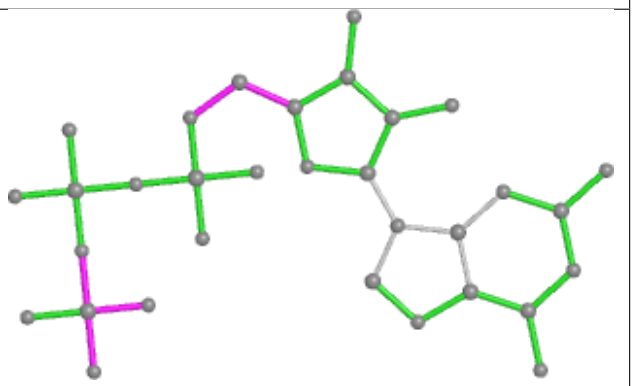

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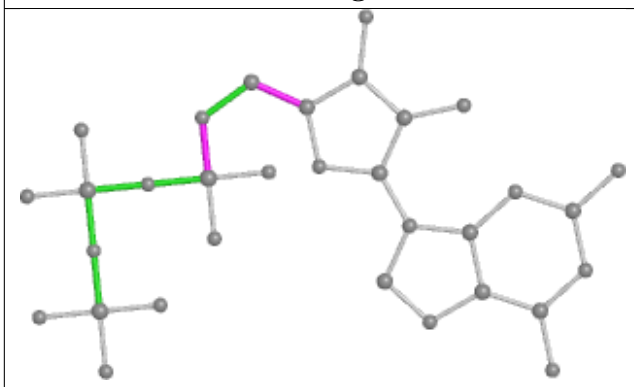

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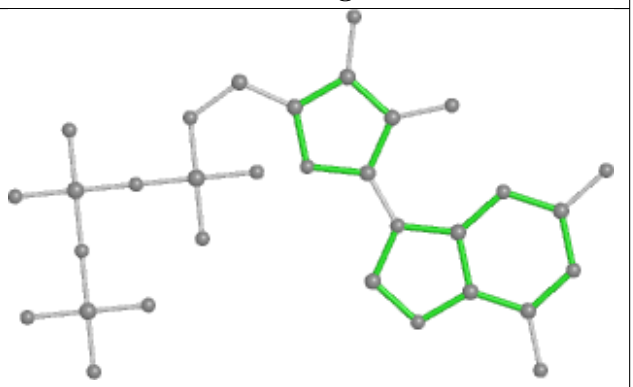
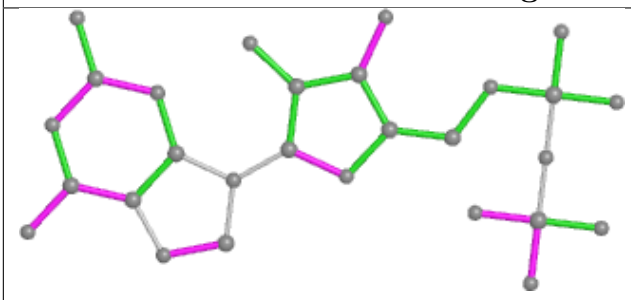


Rings

Ligand GDP D 901



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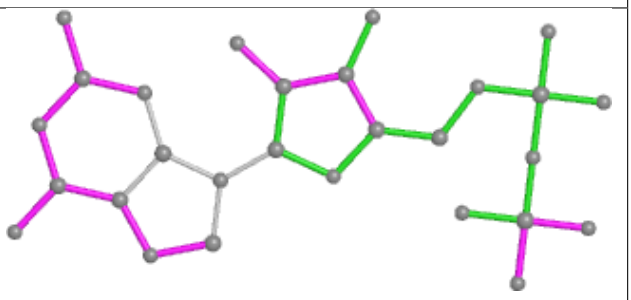

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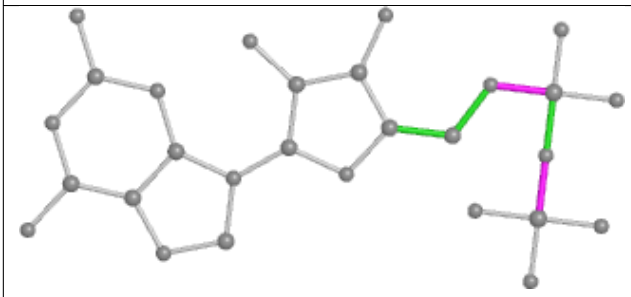

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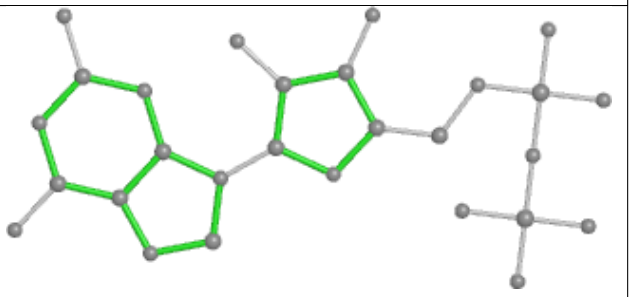
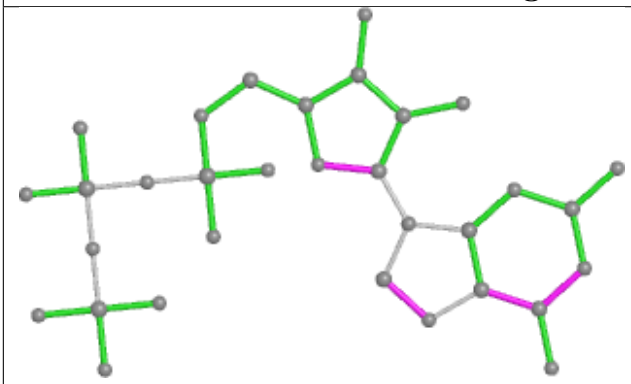


Rings

Ligand GTP C 501



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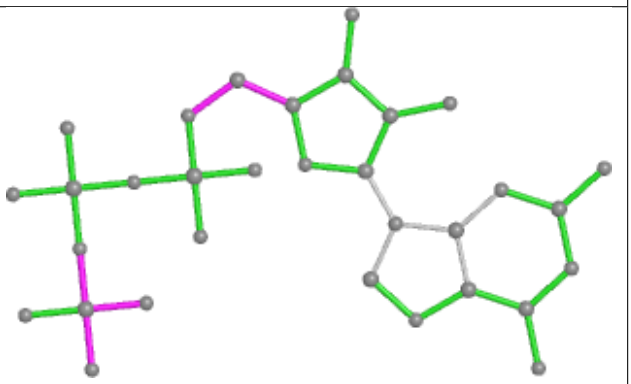

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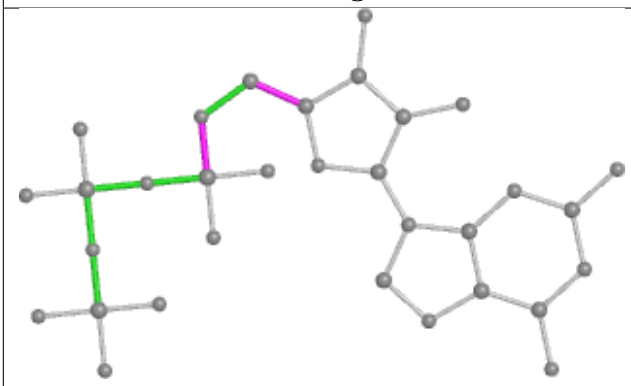

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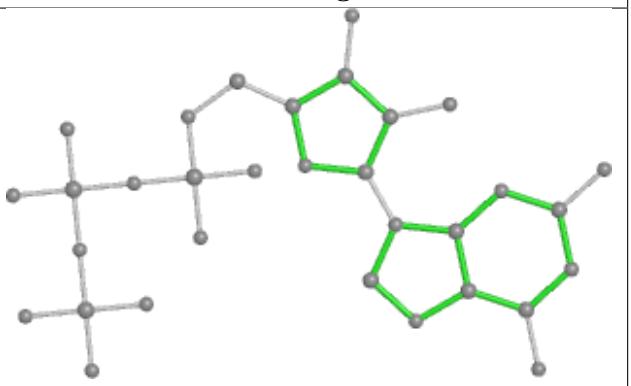
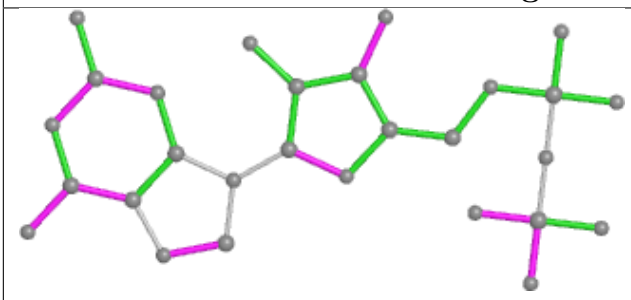


Rings

Ligand GDP B 901



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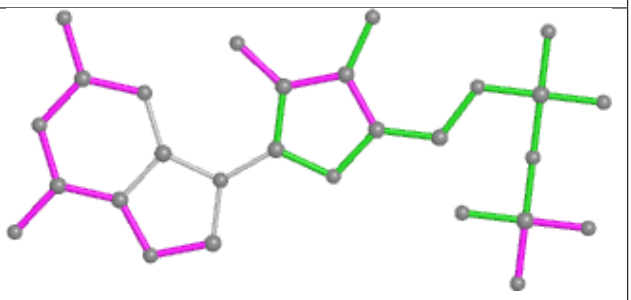
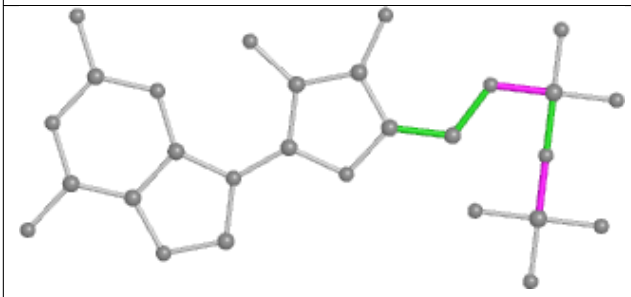
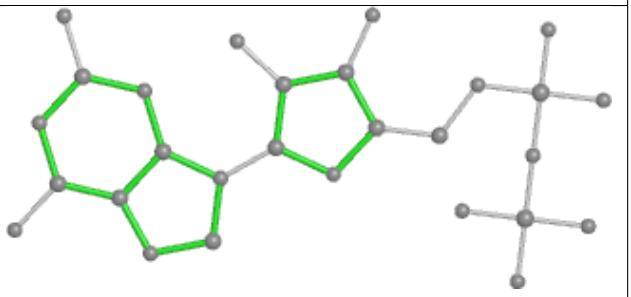


Bond angles

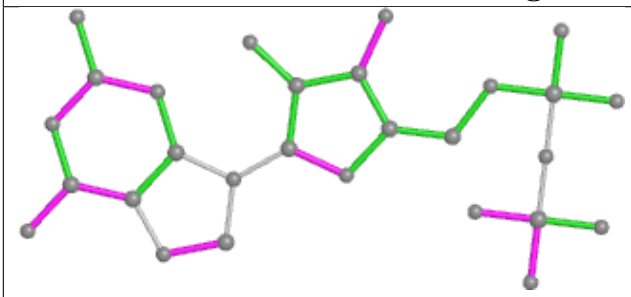


Torsions

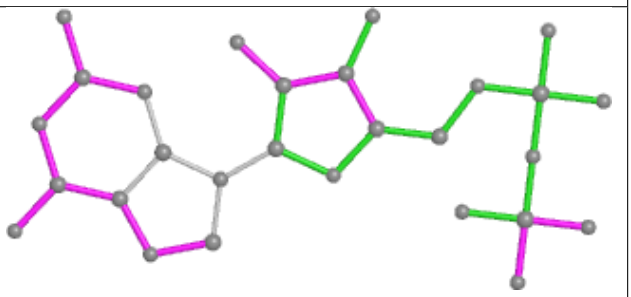


Rings

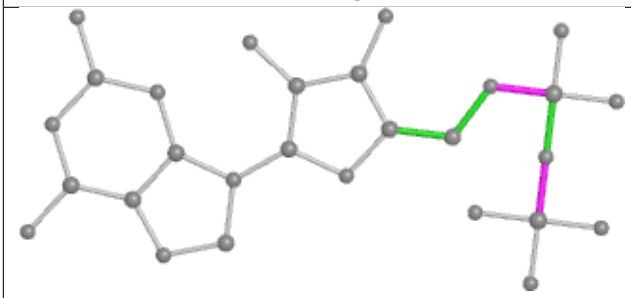
Ligand GDP J 901



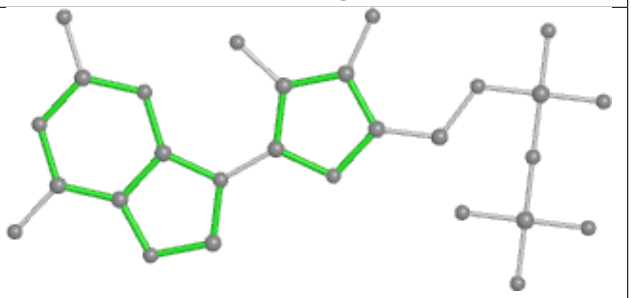
Bond lengths



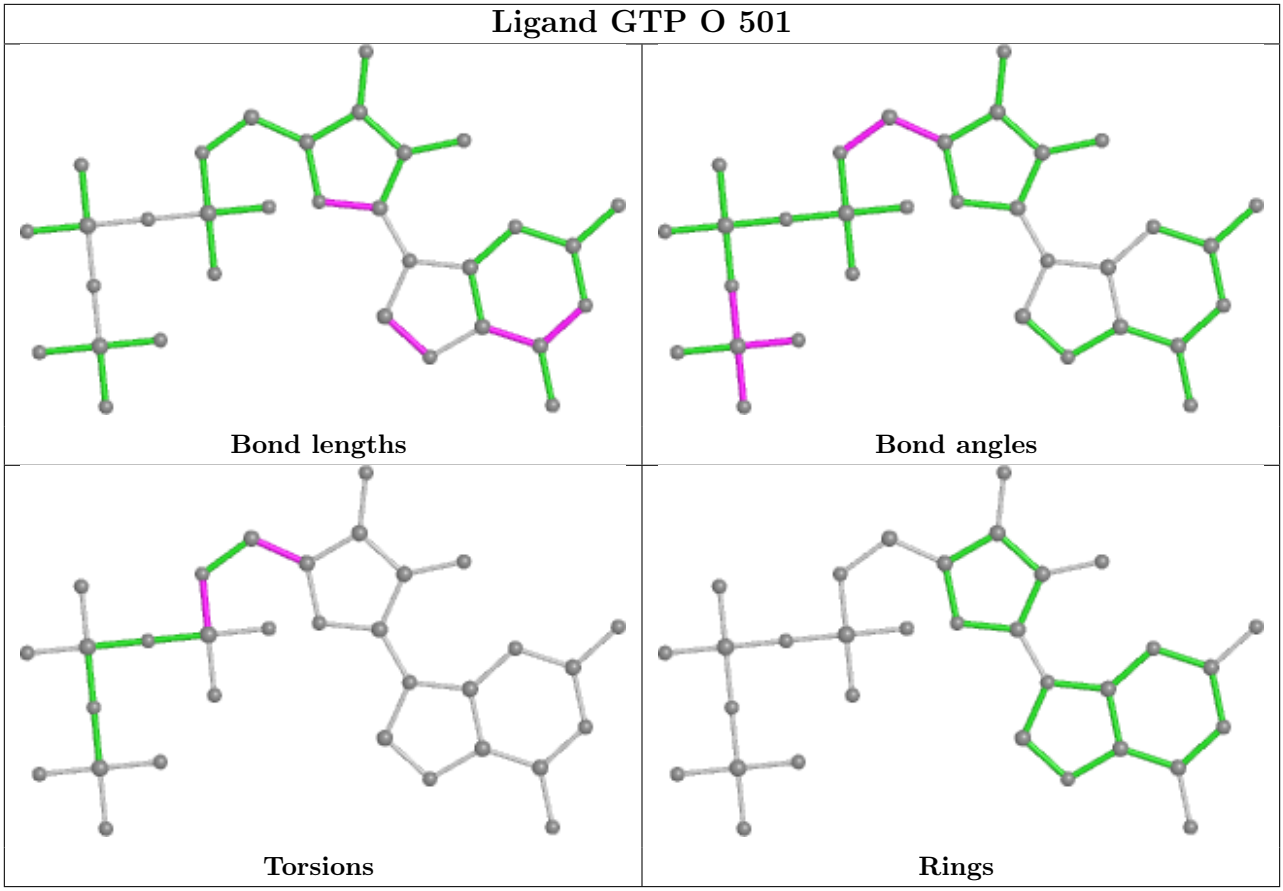
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

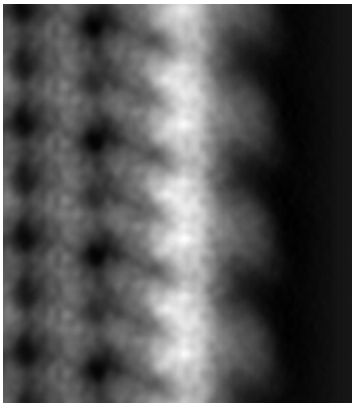
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6782. These allow visual inspection of the internal detail of the map and identification of artifacts.

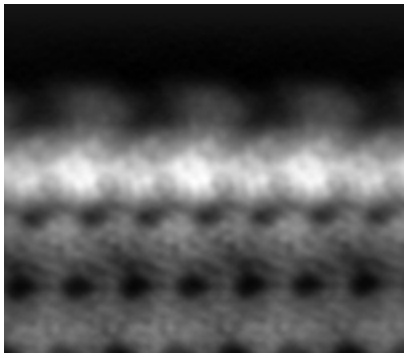
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

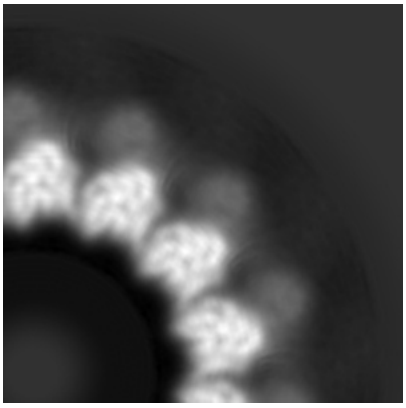
6.1.1 Primary map



X



Y

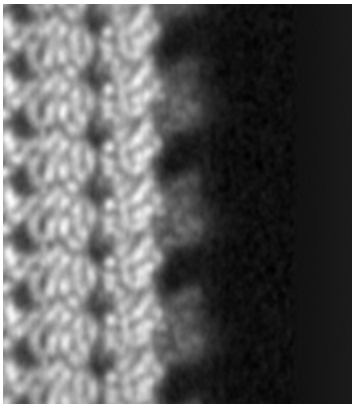


Z

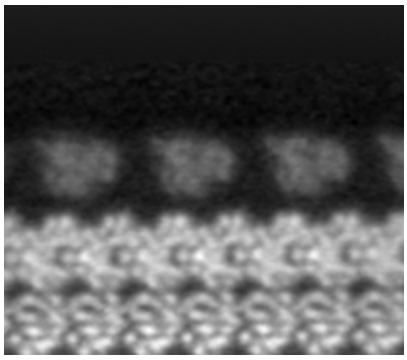
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

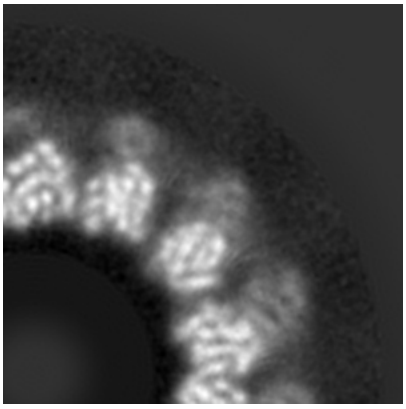
6.2.1 Primary map



X Index: 96



Y Index: 96

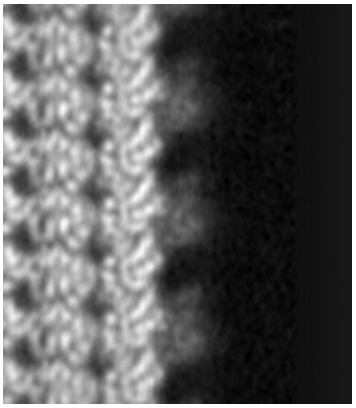


Z Index: 110

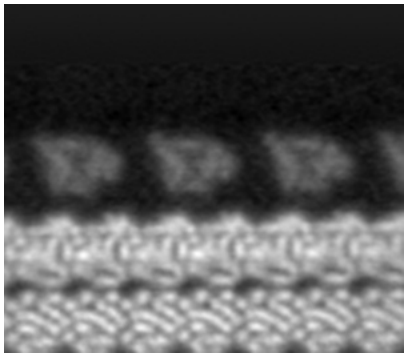
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

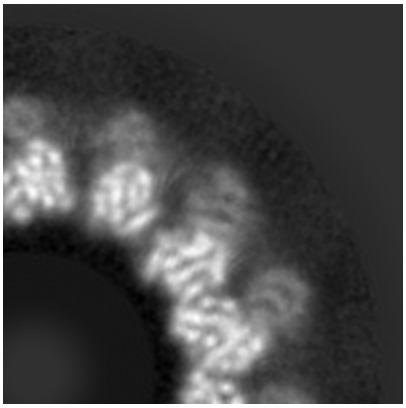
6.3.1 Primary map



X Index: 95



Y Index: 99

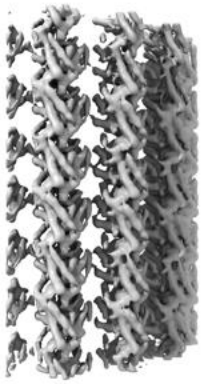


Z Index: 104

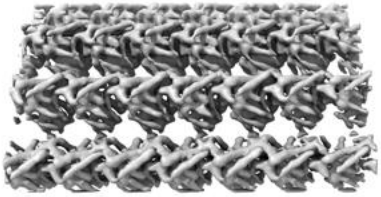
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 7.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

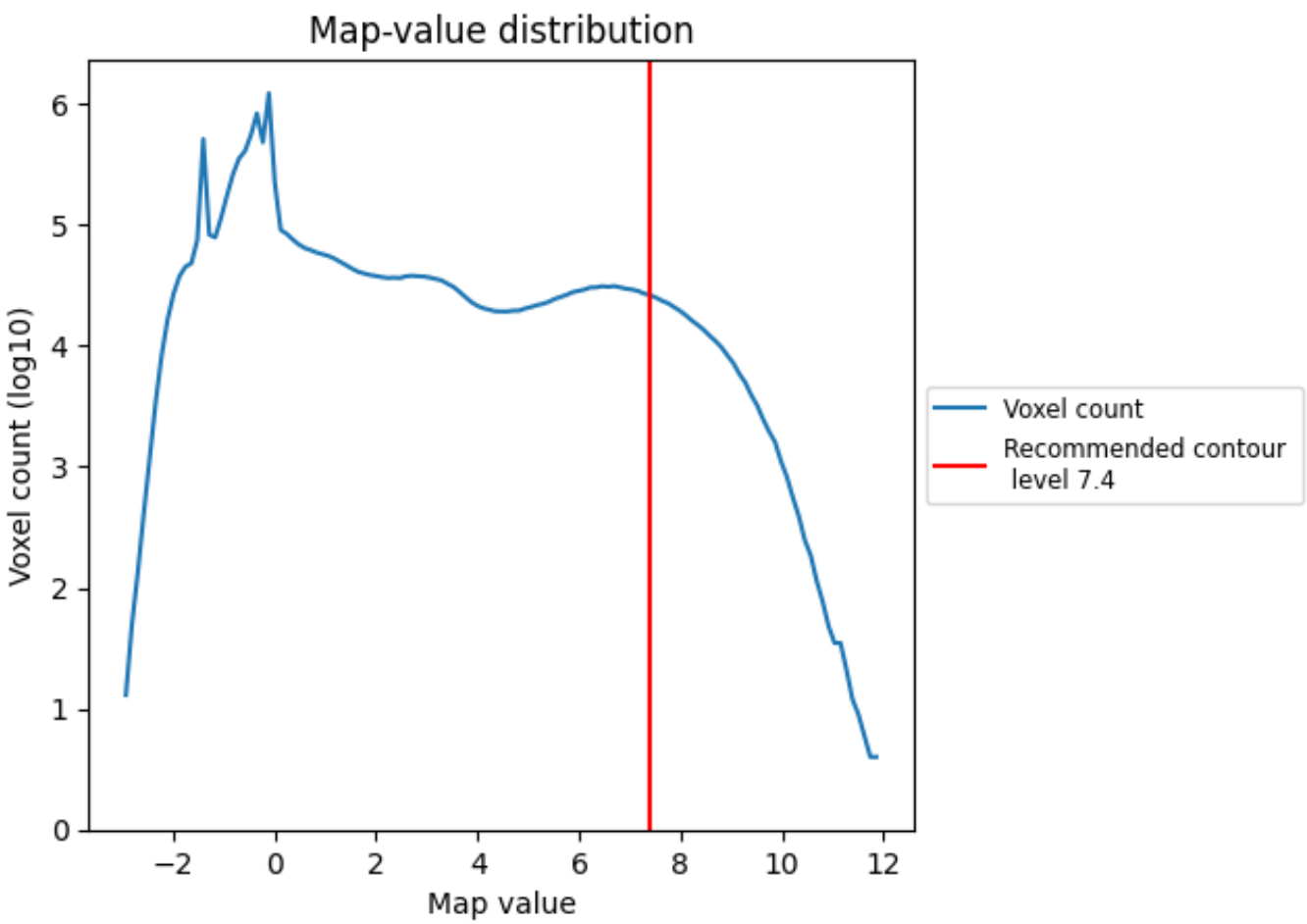
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

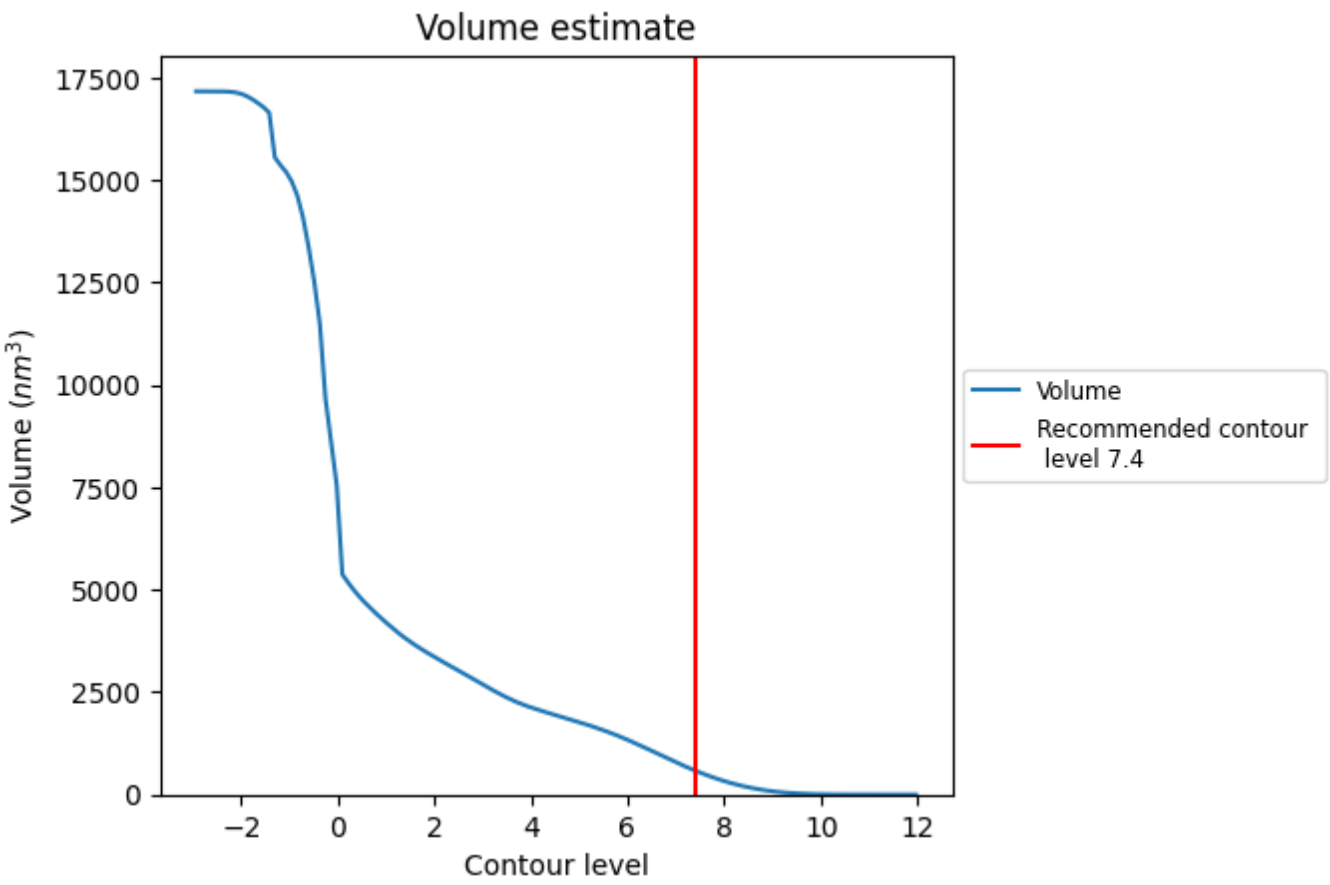
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 586 nm^3; this corresponds to an approximate mass of 529 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

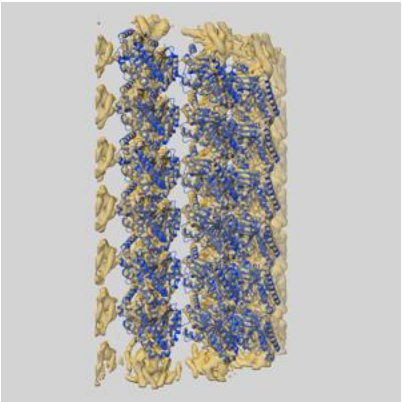
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

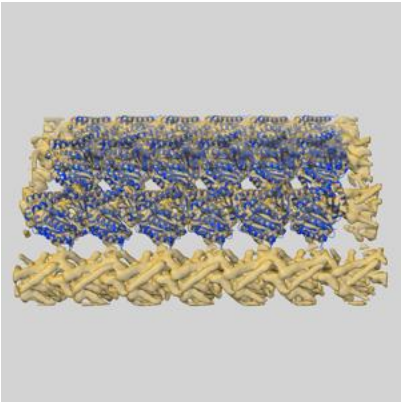
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6782 and PDB model 5XXW. Per-residue inclusion information can be found in section 3 on page 8.

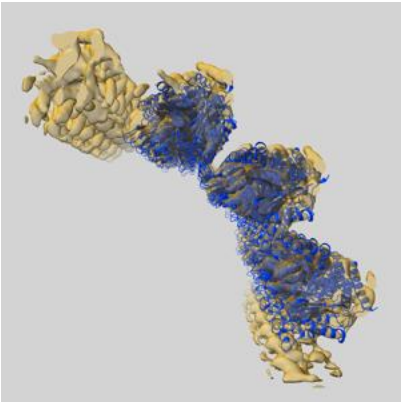
9.1 Map-model overlay (i)



X



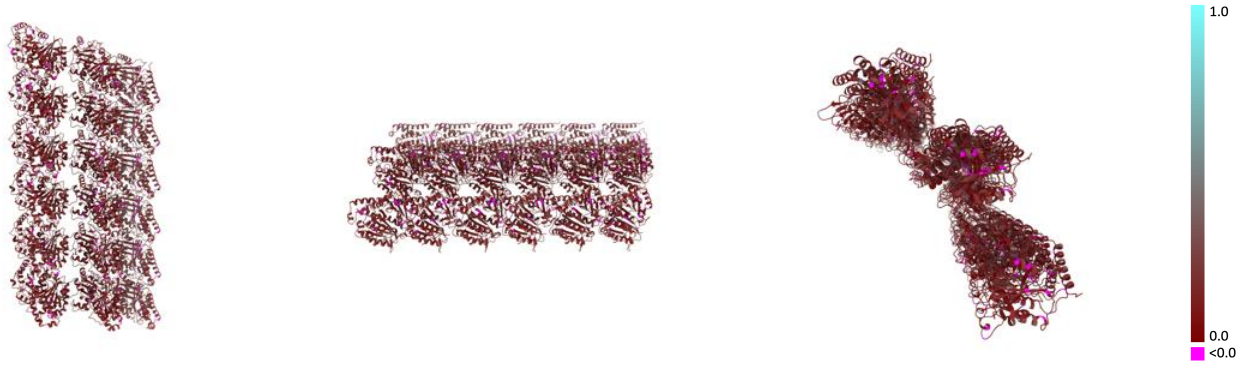
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

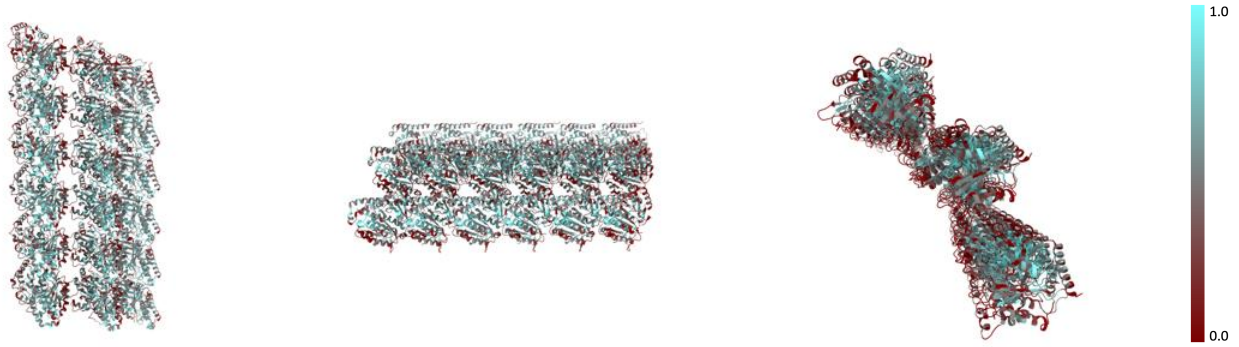
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

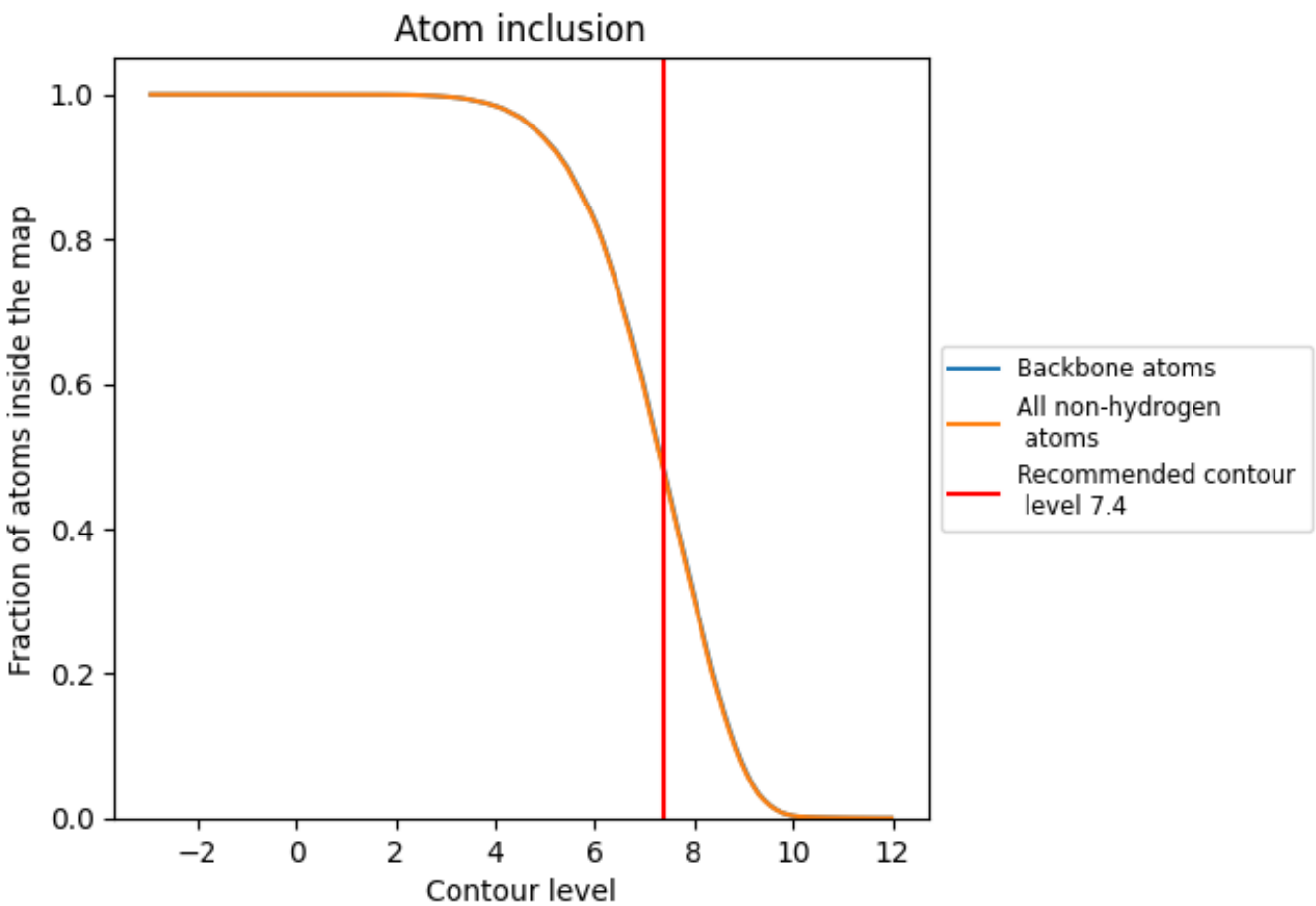
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.4).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (7.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4748	0.1640
A	0.5089	0.1690
B	0.5314	0.1630
C	0.5095	0.1690
D	0.5296	0.1660
E	0.5083	0.1670
F	0.5296	0.1610
G	0.4845	0.1680
H	0.4605	0.1630
I	0.4830	0.1640
J	0.4602	0.1590
K	0.4866	0.1650
L	0.4623	0.1600
M	0.4064	0.1640
N	0.5048	0.1670
O	0.4049	0.1640
P	0.5015	0.1670
Q	0.4104	0.1610
R	0.5012	0.1630